R-08-111

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Site descriptive modelling SDM-Site Laxemar

Birgitta E Kalinowski (editor)
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Preface

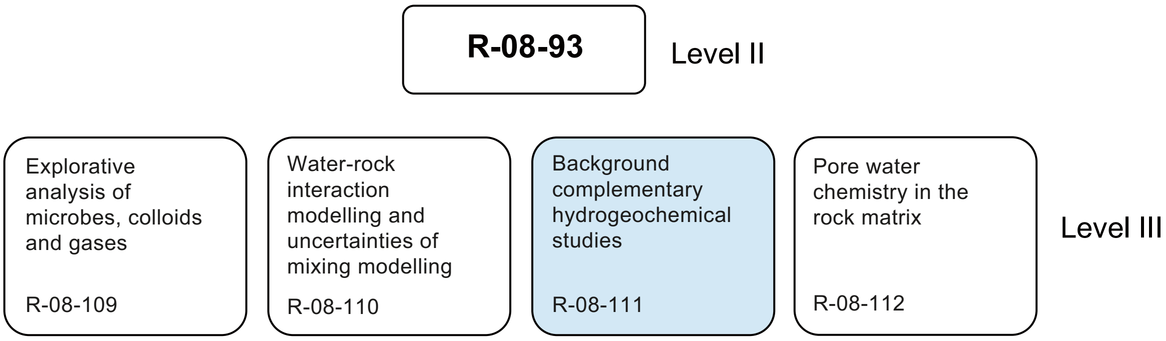
The overall objectives of the hydrogeochemical description for Laxemar are to establish a detailed understanding of the hydrogeochemical conditions at the site and to develop models that fulfil the needs identified by the safety assessment groups during the site investigation phase. Issues of concern to safety assessment are radionuclide transport and technical barrier behaviour, both of which are dependent on the chemistry of groundwater and pore water and their evolution with time.

The work has involved the development of descriptive and mathematical models for groundwaters in relation to rock domains, fracture domains and deformation zones. Past climate changes are the major driving force for hydrogeochemical changes and therefore of fundamental importance for understanding the palaeohydrogeological, palaeohydrogeochemical and present evolution of groundwater in the crystalline bedrock of the Fennoscandian Shield.

Understanding current undisturbed hydrochemical conditions at the proposed repository site is important when predicting future changes in groundwater chemistry. The causes of copper corrosion and/or bentonite degradation are of particular interest as they may jeopardise the long-term integrity of the planned SKB repository system. Thus, the following variables are considered for the hydrogeochemical site descriptive modelling: pH, Eh, sulphur species, iron, manganese, carbonate, phosphate, nitrogen species, total dissolved solids (TDS), isotopes, colloids, fulvic and humic acids and microorganisms. In addition, dissolved gases (e.g. carbon dioxide, methane and hydrogen) are of interest because of their likely participation in microbial reactions.

In this series of reports, the final hydrogeochemical evaluation work of the site investigation at the Laxemar site, is presented. The work was conducted by SKB's hydrogeochemical project group, ChemNet, which consists of independent consultants and university researchers with expertise in geochemistry, hydrochemistry, hydrogeochemistry, microbiology, geomicrobiology, analytical chemistry etc. The resulting site descriptive model version, mainly based on available primary data from the extended data freeze L2.3 at Laxemar (November, 30 2007). The data interpretation was carried out during November 2007 to September 2008. Several groups within ChemNet were involved and the evaluation was conducted independently using different approaches ranging from expert knowledge to geochemical and mathematical modelling including transport modelling. During regular ChemNet meetings the results have been presented and discussed.

The original works by the ChemNet modellers are presented in four level III reports containing complementary information for the bedrock hydrogeochemistry Laxemar Site Descriptive Model (SDM-Site Laxemar, R-08-93) level II report.



There is also a fifth level III report: Fracture mineralogy of the Laxemar area by Sandström et al. R-08-99.

The ChemNet members contributing to this report are (in alphabetic order):

David Arcos, Amphos, Barcelona, Spain (section 2)
Lara Duro, Amphos, Barcelona, Spain (section 2)
Mel Gascoyne, GGP Inc, Pinawa, Canada (section 3 and 5)
Ioana Gurban, 3D-Terra, Montreal, Canada (section 1, 3 and 5)
Jorge Molinero, Amphos, Barcelona, Spain (section 2)
Ann-Chatrin Nilsson, Geosigma AB, Uppsala, Sweden (section 4)
Joaquín Salas, Amphos, Barcelona, Spain (section 2)
John Smellie, Conterra, Sweden (section 6)
Eva-Lena Tullborg, Terralogica, Sweden (section 6)

This report is a compilation of six different projects that have been finished independently of each other.

Section #1: M3 modelling of the hydrochemical parameters of Laxemar-Simpevarp groundwaters by Ioana Gurban.

The focus of this part is on updating the hydrochemical model, to make uncertainty tests and to present the final models that can be integrated better with the hydrodynamic models. M3 modelling helps to summarise and understand the measured data, by using the major elements and the isotopes $\delta^{18}O$ and $\delta^{2}H$ as variables.

The visualisation of the mixing proportions along the boreholes helps to understand the distribution of the data in the domain and to check and compare the results of different models; and therefore to choose the model which best describes the measured data.

Section #2: Integrated hydrogeological and geochemical modelling of the Laxemar-Simpevarp area during the recent Holocene (last 8,000 years) by Jorge Molinero, Joaquín Salas, David Arcos and Lara Duro.

Reactive mixing and reactive solute transport models are used as quantitative tools in order to evaluate how much disturbance can be allowed for a given groundwater sample at repository depth and still meet the SKB suitability criteria. Spatial analysis and 3D visualization of available representative samples in Forsmark was performed. The computed M3 mixing fractions show a spatial distribution qualitatively correlated with key hydrochemical signatures, such as strontium (for Deep Saline), magnesium (for Littorina), $\delta^{18}O$ and $\delta^{2}H$ (for Glacial) and tritium (for Modified meteoric).

Section #3: Application of the Drilling Impact Study (DIS) to Laxemar groundwaters by Mel Gascoyne and Ioana Gurban.

In the Drilling Impact Study (DIS) project a tracer is used as an indicator of contamination to attempt to correct the groundwater composition for dilution or contamination by surface waters. By calculating the drilling water volume lost in the fractures during drilling, it is possible to determine how much water should be pumped out from the section before sampling.

Section #4: Laxemar site investigation: Quality of hydrochemical analyses (DF version 2.3) by Ann-Chatrin Nilsson.

There is high confidence in the set of major constituents for each sample. Independent methods were used to check the consistency of the major ions and to confirm the concentrations of chloride, sulphate, bromide and iron. The bromide analyses were found to be more uncertain than most other major ions.

Section #5: Determination of residence time: ^{4}He and ^{36}Cl in Laxemar groundwaters by Mel Gascoyne and Ioana Gurban.

Helium-4 and ^{36}Cl are useful isotopic tracers for determining the residence time of groundwater for identifying mixing of groundwaters and the characteristics of water-rock interaction. This section describes the results of ^{4}He and ^{36}Cl analyses of selected groundwater types at the Laxemar-Simpevarp area to determine if the data support the proposed Littorina origin of this high Mg-SO_4 type of groundwater. Comparison is made with results from the other sites.

Section #6: Quality assurance and categorisation of groundwater samples from the Laxemar-Simpevarp area by John Smellie and Eva-Lena Tullborg.

Documentation of the percussion boreholes is presented in tabular form showing the major category criteria that characterise the groundwater chemistry from each sampled borehole length or isolated borehole section. The cored borehole documentation includes the groundwater category table for each sampled borehole section accompanied by a brief description of the hydraulic character of the borehole and the packed-off sections samples, the hydrochemistry of the drilling water, the major ion and isotope chemistry of the sampled groundwaters and the main reasons to the different categories selected.

Contents

Section 1

M3 modelling of the hydrochemical parameters of Laxemar-Simpevarp groundwaters

Ioana Gurban
3D-Terra

Contents

1 Introduction

This report presents the results of the water classification, mixing modelling and 2D visualisation along boreholes of SDM-Site Laxemar groundwater data obtained from the Extended Data freeze Laxemar 2.3. The focus is on updating the hydrochemical model, to make uncertainty tests and to present the final M3 model that can be better integrated with the hydrodynamic models. The boreholes (cored boreholes and percussion boreholes) that have contributed to the present analysis are: HAS02, HAS03, HAS05, HAS06, HAS07, HAS13, KAS02, KAS03, KAS04, KAS06, HAV04, HAV05, HAV06, HAV07, KAV01, KAV04A, HLX01, HLX03, HLX06, HLX07, HLX10, HLX14, HLX20, HLX21, HLX22, HLX23, HLX24, HLX28, HLX30, HLX33, HLX34, HLX35, HLX37, HLX38, HLX39, KLX01, KLX02, KLX03, KLX04, KLX05, KLX06, KLX07A, KLX08, KLX09, KLX10, KLX11A, KLX12A, KLX13A, KLX15A, KLX17A, KLX18A, KLX19A, KLX20A, KLX21B, HSH02, HSH03, KSH01A, KSH02 and KSH03A. The complete data set used is presented in Appendix 1. A map with the location of the boreholes can be found in /Laaksoharju et al. 2009/.

The need for additional uncertainty tests was identified during the previous Laxemar modelling phases and issues such as the use of different end-members are addressed. In order to show examples of the tests done, the Laxemar 2.2 modelling is presented in Appendix 2. Several models were tested. The model that best fits the conceptual model and the hydrogeochemical understanding is presented in this report. For a proper comparison of the Laxemar and Forsmark sites, the same methodology was used at both sites.

2 M3 modelling

2.1 Data selection

The M3 method consists of 4 steps: a standard principal component analysis (PCA), selection of reference waters, calculations of mixing proportions, and, finally, mass balance calculations (for more details see /Laaksoharju 1999, Laaksoharju et al. 1999 and Gómez et al. 2006/).

The SDM-Site Laxemar data were analysed in the different phases (Simpevarp 1.2 and then Laxemar 1.2 and Laxemar 2.1) with different versions of the M3 code. The old M3 2D version /Laaksoharju 1999/ was updated and hyperspace calculations are now possible. The new version /Gómez et al. 2006/ of M3 makes possible the calculations in 2PC or n-PC (n principal components, where n is the number of end-members of the model). Several runs were made with the new version of M3 in the SDM-Site Laxemar 2.1 stage, where the code was extensively tested. This helped to verify that the new M3 2D works exactly like the old M3 code, and then to compare and judge the benefits or limitations by using 2D or n-PC calculations. In general, in the 2D calculations, more data can be included. When using the n-PC calculations, less data are included but the predictions of the conservative elements fit better with the measured values. Therefore, in this report, only the M3 n-PC version is used. Several versions of M3 were tested during the previous exercises and the final version is used here (M3 beta 9).

For the Simpevarp 1.1 stage /Laaksoharju 2004/, 2 models were built: regional and local scale. 113 samples from Simpevarp met the M3 criteria (data for major elements and isotopes) and were used in the M3 modelling. These samples were from boreholes (cored and percussion), soil pipes, lake water, stream water and precipitation. In the Simpevarp 1.2 stage (applied on data from Simpevarp area), version 1.1 was up-dated with the newly available data. For Simpevarp 1.2 phase, 2 models were also built: regional and local scale. 326 samples from Simpevarp met the M3 criteria (data for major elements and isotopes) and were used in the M3 modelling. These samples were from boreholes (cored and percussion), soil pipes, lake water, stream water and precipitation. From the 326 samples available, 180 were considered representative from the hydrochemical point of view and 146 non-representative. The Simpevarp local scale model area (Laxemar 1.2, /SKB 2006a/) exercise employed the data from the Simpevarp 1.2 model and the data available at Laxemar site. From the 355 samples available, 175 were considered representative from the hydrochemical point of view. The SDM-Site

Laxemar 2.1 /SKB 2006b/ M3 modelling employed only groundwater data, from percussion and cored boreholes, meaning 205 groundwater samples. From the 205 samples, 59 were considered representative from the hydrochemical point of view and 146 non representative.

The Laxemar 2.2 M3 model employed a total of 397 samples, from percussion and cored boreholes. From these samples, 77 are considered representative.

The SDM-Site Laxemar 2.3 dataset used in M3 consists of 473 groundwater samples, from which 103 are considered representative, following the QA guidelines in /Laaksoharju et al. 2009/. All the data used in the Laxemar 2.3 M3 modelling are presented in SKB database Simon.

2.2 End-members

The end-members are the most extreme-composition waters present in the hydrogeochemical system studied (here SDM-Site Laxemar). The end-members can be samples from the site or modelled extreme-composition waters, defined by expert judgement after a hydrogeochemical evaluation of the site (as per /Gimeno et al. 2009/). The following reference waters were used in the M3 modelling (for analytical data see Table 2-1):

- **Deep Saline end-member:** Brine type of reference water, represents the deep brine type (Cl = 47,000 mg/l) of water sampled from borehole KLX02: 1,631–1,681 m /Laaksoharju et al. 1995/. An old age for the Deep Saline is suggested by the measured ^{36}Cl values indicating a minimum residence time of 1.5 Ma for the Cl component /Laaksoharju and Wallin 1997/.
- **Glacial end-member:** Represents a possible melt-water composition from the last glaciation > 11,000 BC. Modern glacial melt water from Norway was used for the major elements and the δ^{18}O isotope value (−21‰ SMOW) was based on measured values of δ^{18}O in calcite surface deposits /Tullborg and Larson 1984/. The δ^{2}H value (−158‰ SMOW) is a modelled value based on the global relationship ($\delta^{2}H = 8 \times \delta^{18}O + 10$) for the meteoric water line.
- **Old Meteoric-Glacial end-member:** In order to better predict the δ^{18}O values, a mixture of Old Meteoric-Glacial type of water was used as an end-member. This water has $\delta^{2}H = -118‰$ and $\delta^{18}O = -16‰$. This end-member is used as an alternative model instead of the glacial end-member, see chapter 6 in this report.
- **Littorina Water end-member:** Represents modelled Littorina water (see Table 2-1). The Littorina composition is more saline than the current Baltic sea composition. Therefore Littorina water is used in the calculations.
- **Altered meteoric end-member:** Corresponds to an upper bedrock water composition, obtained by the infiltration of meteoric water (the origin can be rain or snow) in the bedrock. The composition of the sample HLX28 (10231) was used as the end-member. In the Laxemar 2.2 modelling exercise, another shallow end member was identified. This sample was from HLX05 (sample number 2558) but it was an experimental water, which was later deleted from Sicada, therefore it was decided to not use it in the final modelling. The final choice was HLX28 which has a high HCO_3^- (265 mg/l) and a low Cl (23 mg/l) concentration. This sample is taken from 80 m depth, representing well the upper bedrock.

Table 2-1. Groundwater analytical or modelled data (Littorina and old meteoric-glacial) used as end-members in the M3 modelling for Laxemar 2.3.

End Member	ID Code	Cl (mg/l)	Na (mg/l)	K (mg/l)	Ca (mg/l)	Mg (mg/l)	HCO3 (mg/l)	SO4 (mg/l)	d2H‰	d18O‰
Deep saline	Laxemar SGKLX02	47,200	8,200	45.5	19,300	2.12	14.1	10	–44.9	–8.9
Glacial		0.5	0.17	0.4	0.18	0.1	0.12	0.5	–158	–21
Old meteoric-Glacial		0.5	0.17	0.4	0.18	0.1	0.12	0.5	–118	–16
Littorina Sea		6,500	3,674	134	151	448	92.5	890	–37.8	–4.7
Altered meteoric	HLX28 (10231)	23	110.0	2.97	11.2	3.6	265.00	35.80	–76.5	–10.9

Several tests were made with different shallow end-member compositions and some of these tests are presented in Appendix 2. The final end-members used are the Deep Saline, Glacial, Littorina, and Altered Meteoric HLX28 (10231) as these waters can explain most of the samples from Laxemar.

2.3 The final model (model 1)

The M3 code is applied to the Extended Data freeze Laxemar 2.3 bedrock data, using as variables the major elements and δ^2H and $\delta^{18}O$, and as end-members, Littorina, Altered meteoric (which is sample 10231 from HLX28), Deep Saline (formerly Brine) and Glacial. Previous tests made for Simpevarp and Laxemar earlier datasets showed that the conservative variables (Cl and $\delta^{18}O$) do not give an unique solution, therefore the non conservative species Na, K, Ca, Mg, HCO_3 and SO_4 are included in the calculations.

Several models were studied for Laxemar with different end-members and different variables. In this report the final model with the previously selected end-members and with the complete Laxemar 2.3 dataset is presented. In Appendix 1, alternative models, such as different options for the shallow end member, are presented.

The PCA applied on the SDM-Site Laxemar 2.3 data is illustrated in Figure 2-1. A total of 473 groundwater samples from Laxemar 2.3 were used for this plot. The PCA in Figure 3-1 shows surface water affected by seasonal variation (winter – summer precipitation), a marine trend showing Baltic Sea water influence and, for some Äspö samples, a possible Littorina sea water influence. A glacial and finally a deep groundwater trend are also shown.

The L2.3 dataset and L2.3 representative samples are plotted separately in order to show the distribution of the representative samples. The figure shows that representative samples can describe the data in the same way as the totality of the samples, having the same distribution.

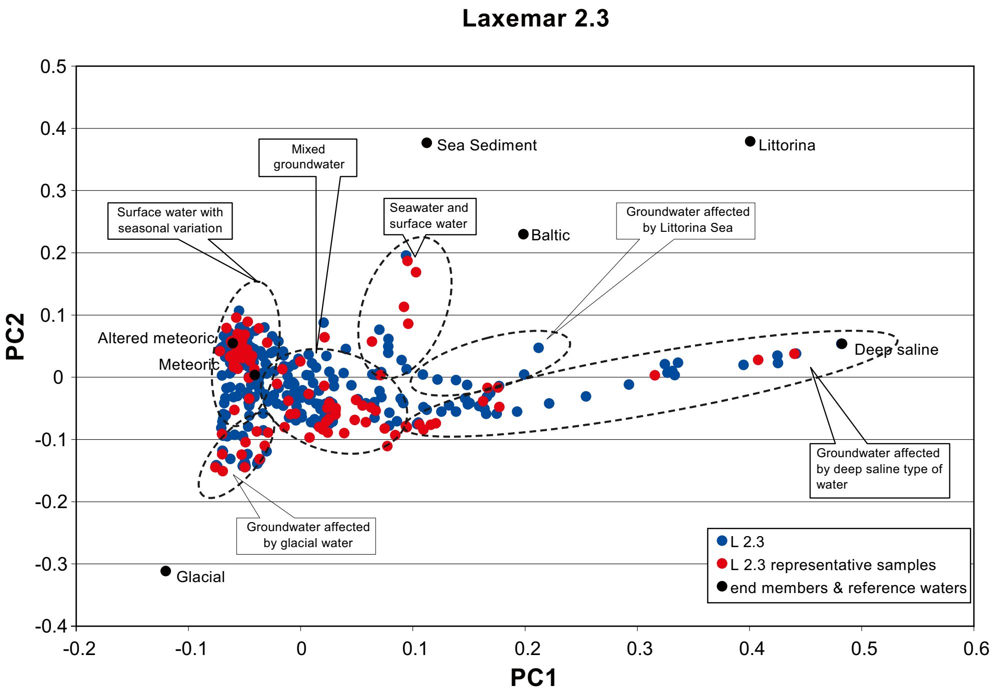


Figure 2-1. Results of principal component analysis and the identification of the reference waters for the Laxemar 2.3 data set. The first principal component accounted for 0.50 of the variance, the first and second principal components, 0.76, and the first, second and third principal components, 0.91. The coverage is 93.5% in n-PC and 84.2% in 2D. All the major elements, $\delta^{18}O$ and δ^2H are used as variables. The Littorina, Deep Saline, Glacial and Altered Meteoric (HLX28, 10231) reference waters are used as end-members for the modelling. The model uncertainty is ± 10%.

3 2D visualisation of the Cl, δ^{18}O, TDS and mixing proportions of the cored boreholes

Figures 3-1 to 3-14 show the Cl, δ^{18}O, TDS and mixing proportions calculated along the cored boreholes with the M3 code. Only the representative samples are shown.

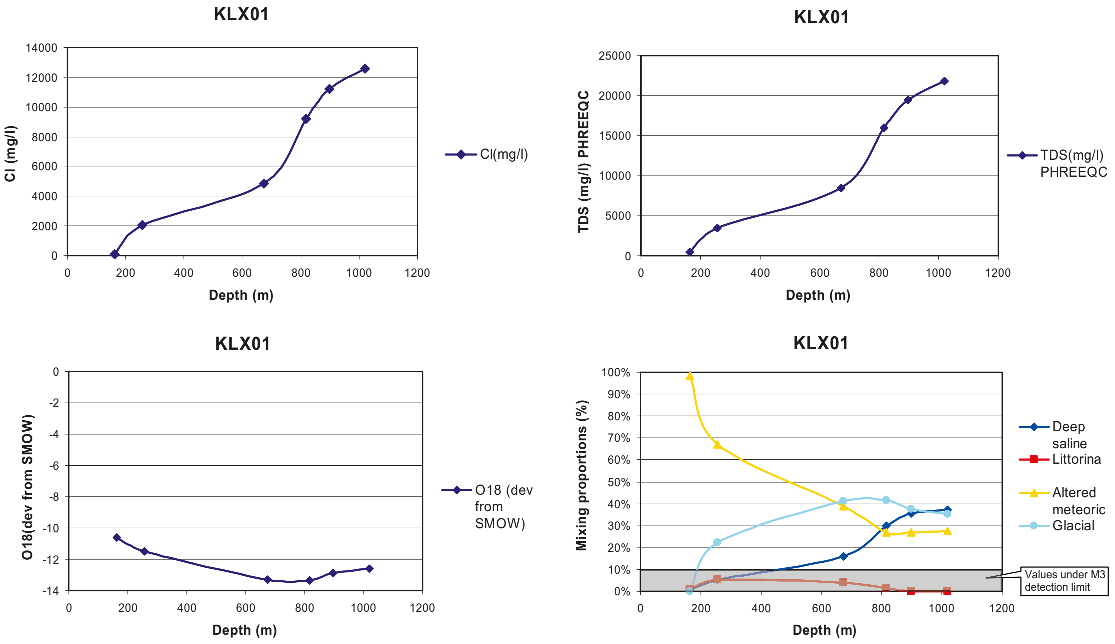


Figure 3-1. Cl, TDS, δ^{18}O, and mixing proportions along KLX01.

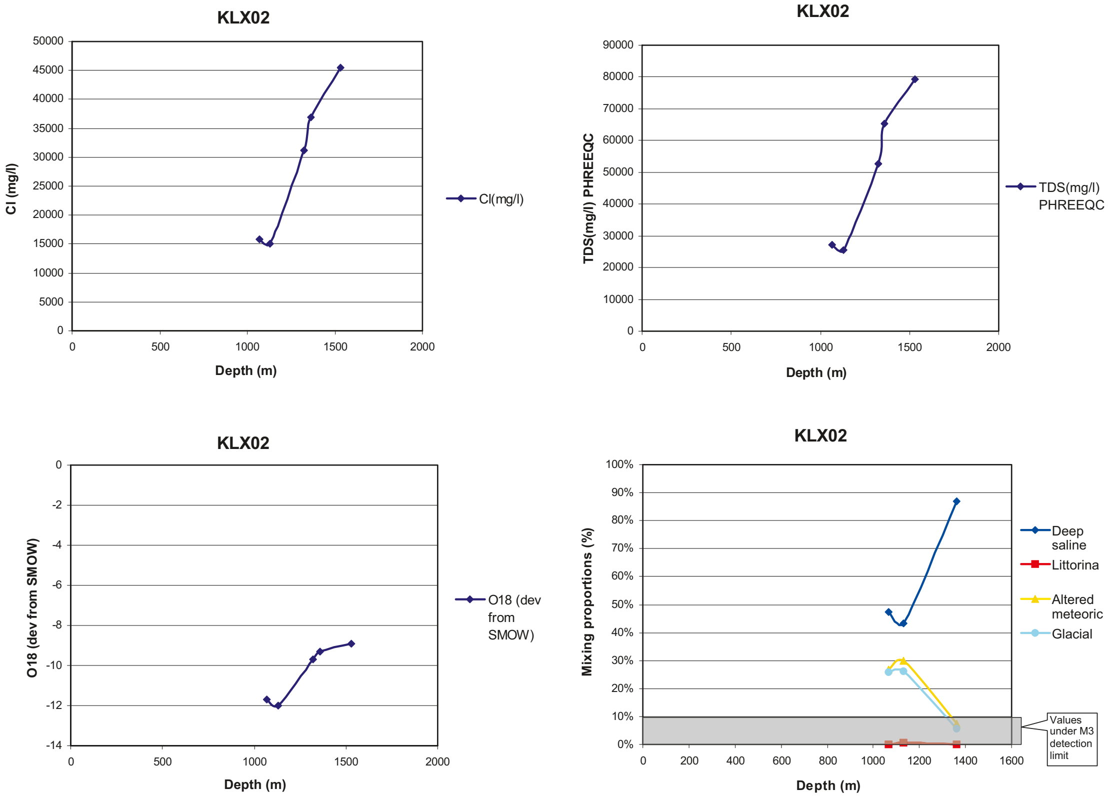


Figure 3-2. Cl, TDS, δ^{18}O, and mixing proportions along KLX02.

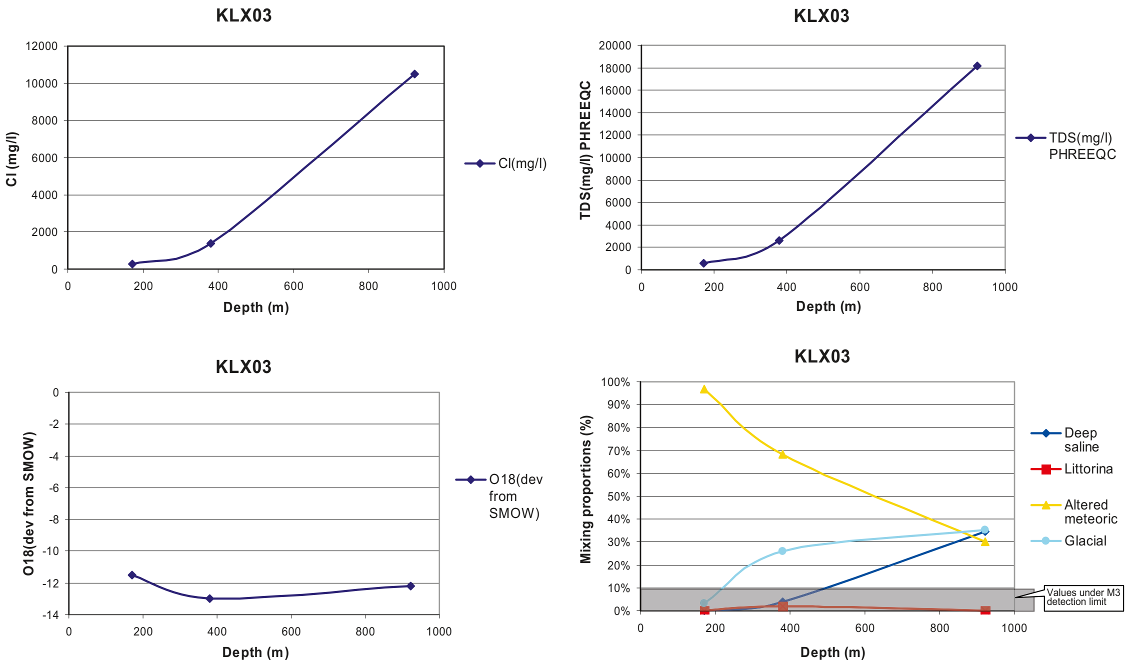


Figure 3-3. Cl, TDS, $\delta^{18}O$, and mixing proportions along KLX03.

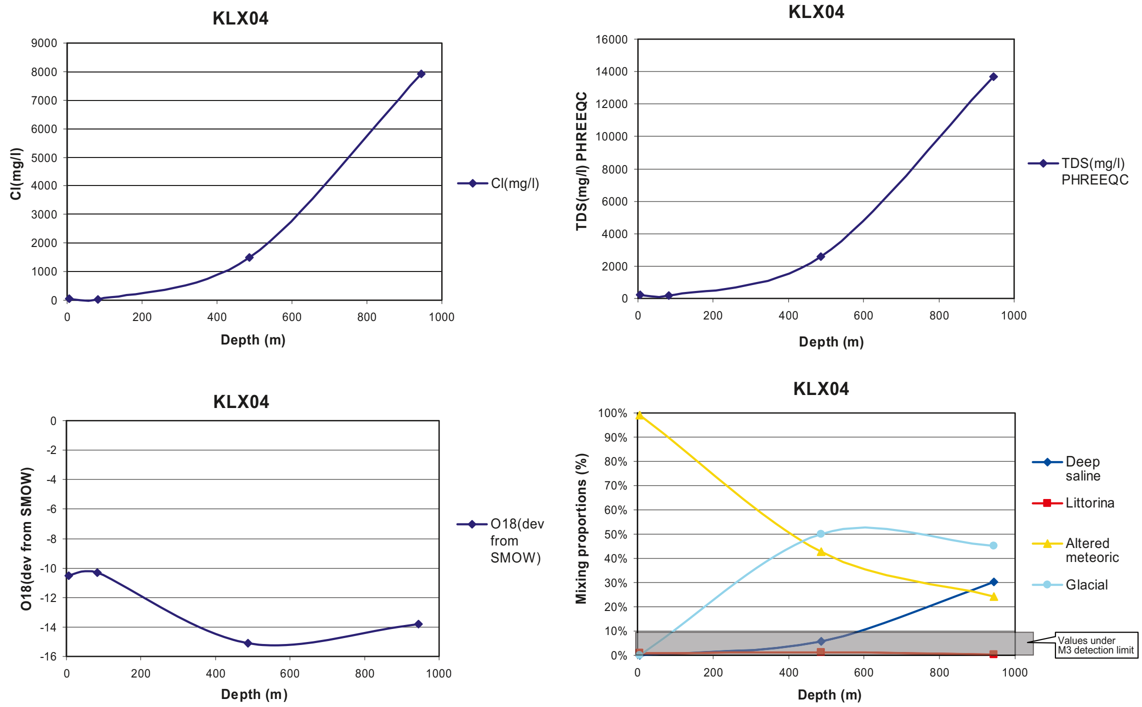


Figure 3-4. Cl, TDS, $\delta^{18}O$, and mixing proportions along KLX04.

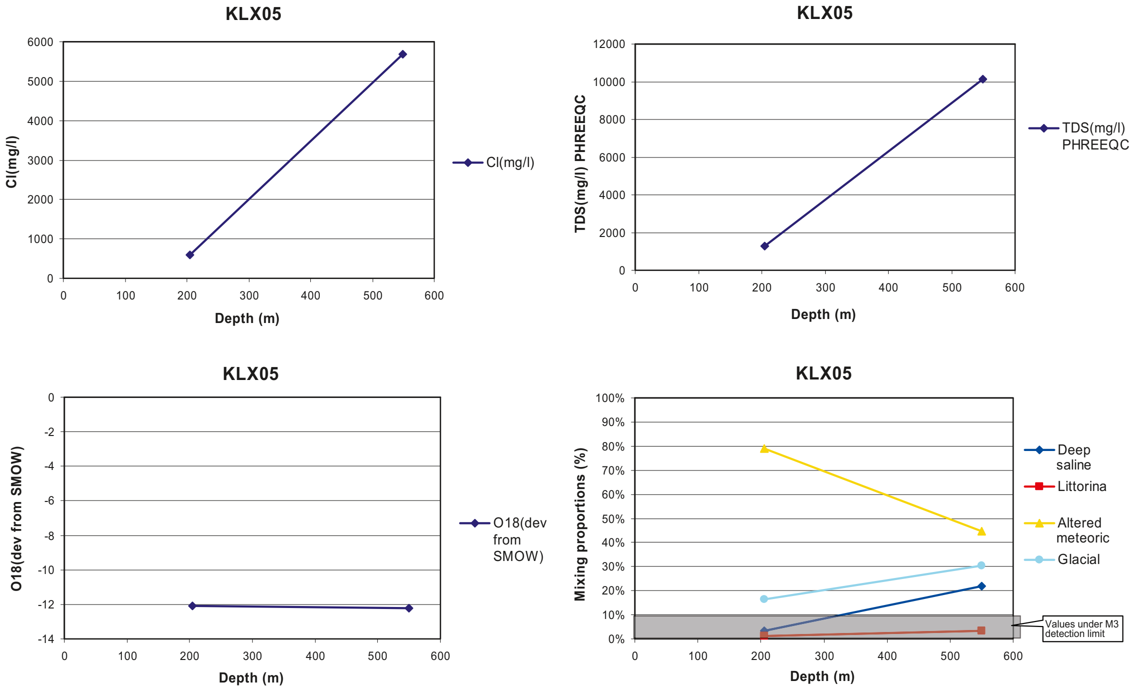


Figure 3-5. *Cl, TDS, δ*^{18}*O, and mixing proportions along KLX05.*

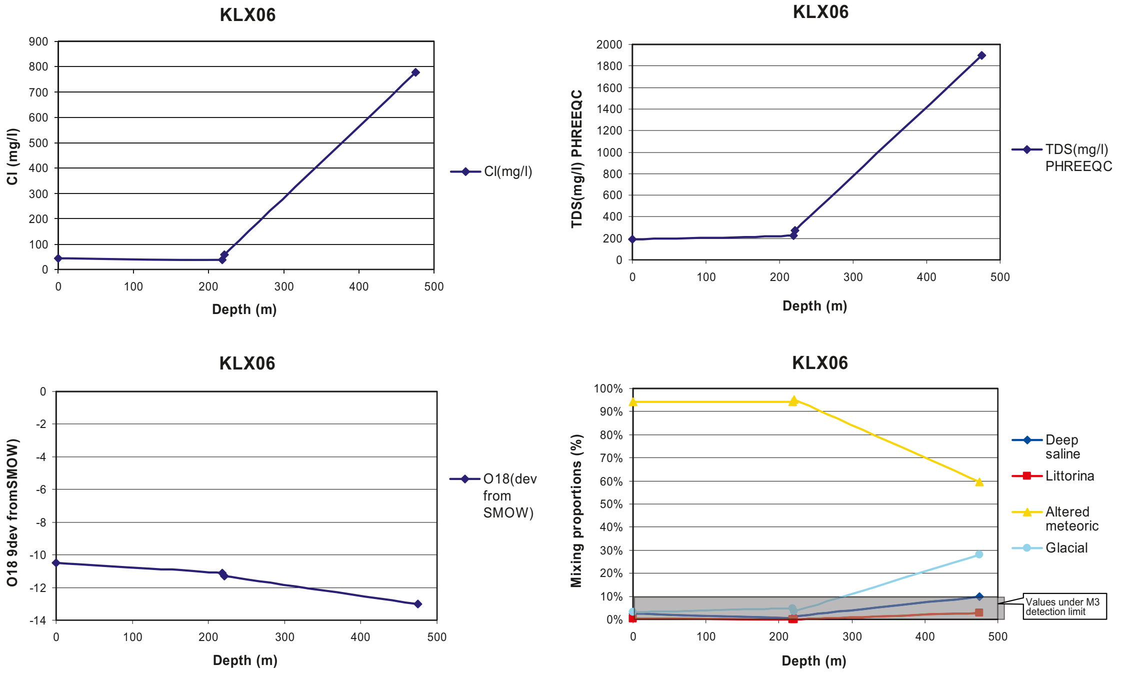


Figure 3-6. *Cl, TDS, δ*^{18}*O, and mixing proportions along KLX06.*

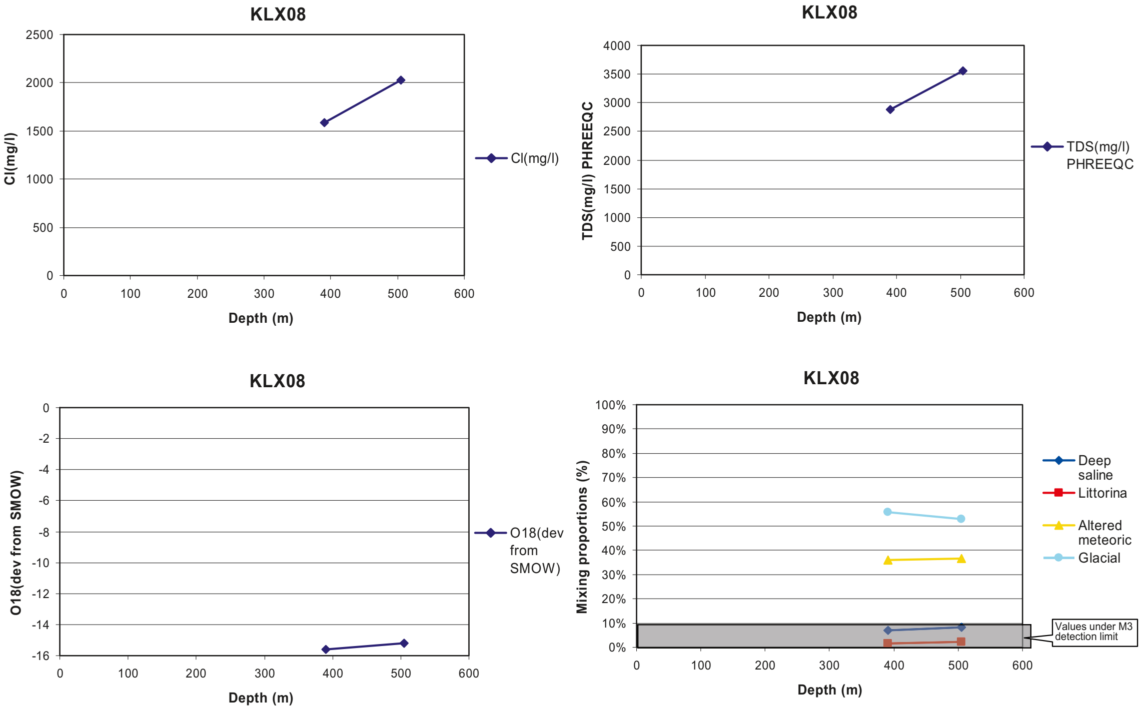


Figure 3-7. Cl, TDS, δ^{18}O, and mixing proportions along KLX08.

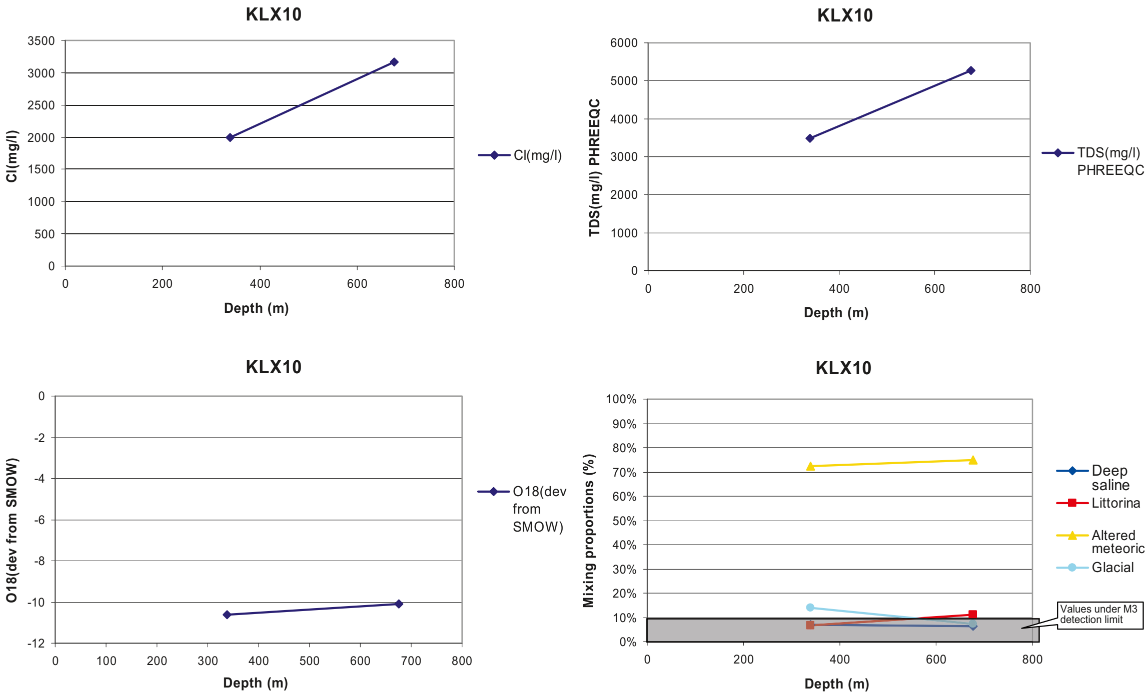


Figure 3-8. Cl, TDS, δ^{18}O, and mixing proportions along KLX10.

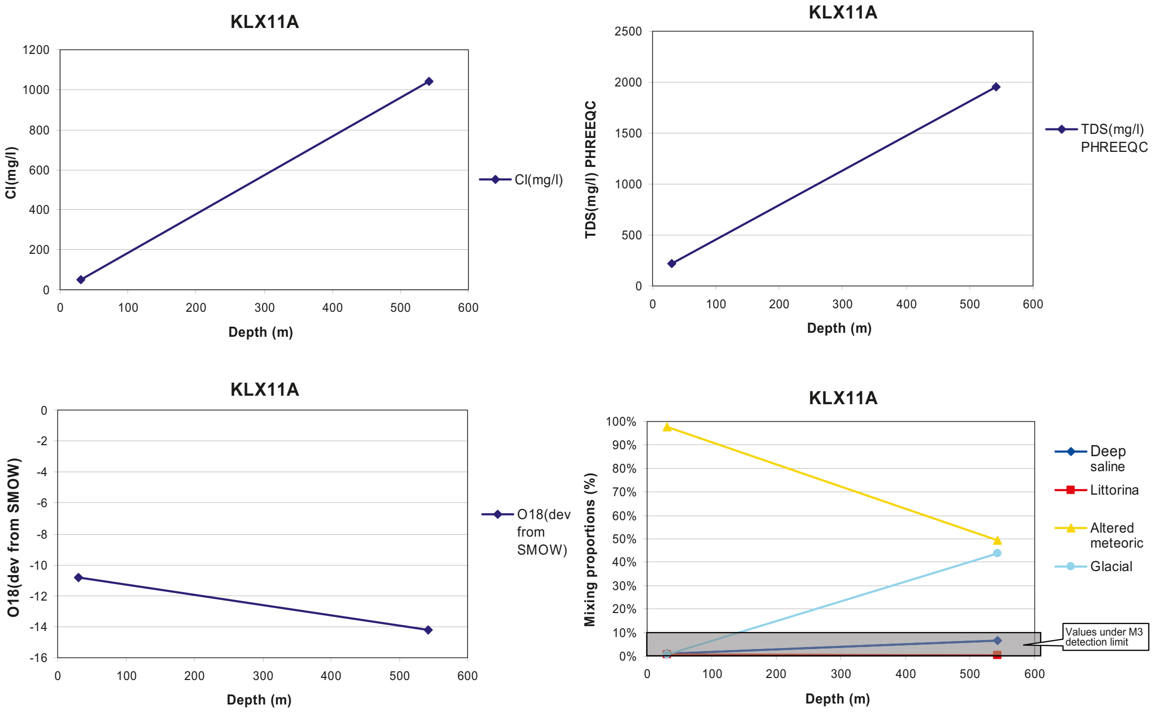


Figure 3-9. Cl, TDS, $\delta^{18}O$, and mixing proportions along KLX11A.

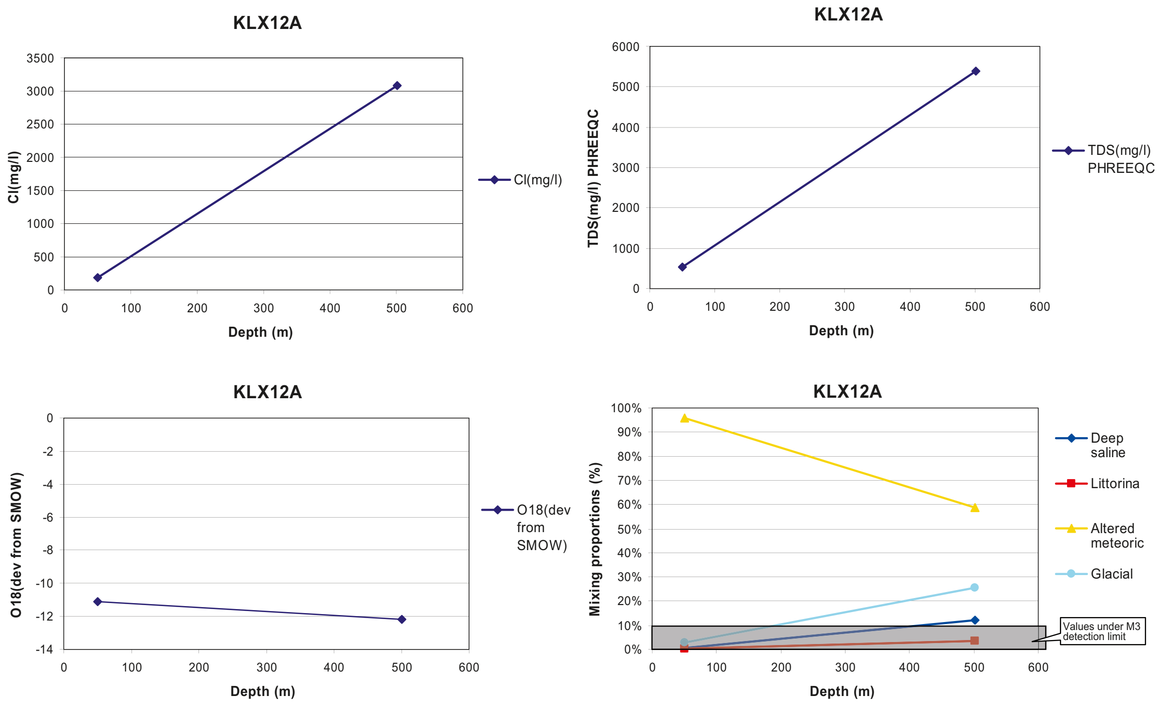


Figure 3-10. Cl, TDS, $\delta^{18}O$, and mixing proportions along KLX12A.

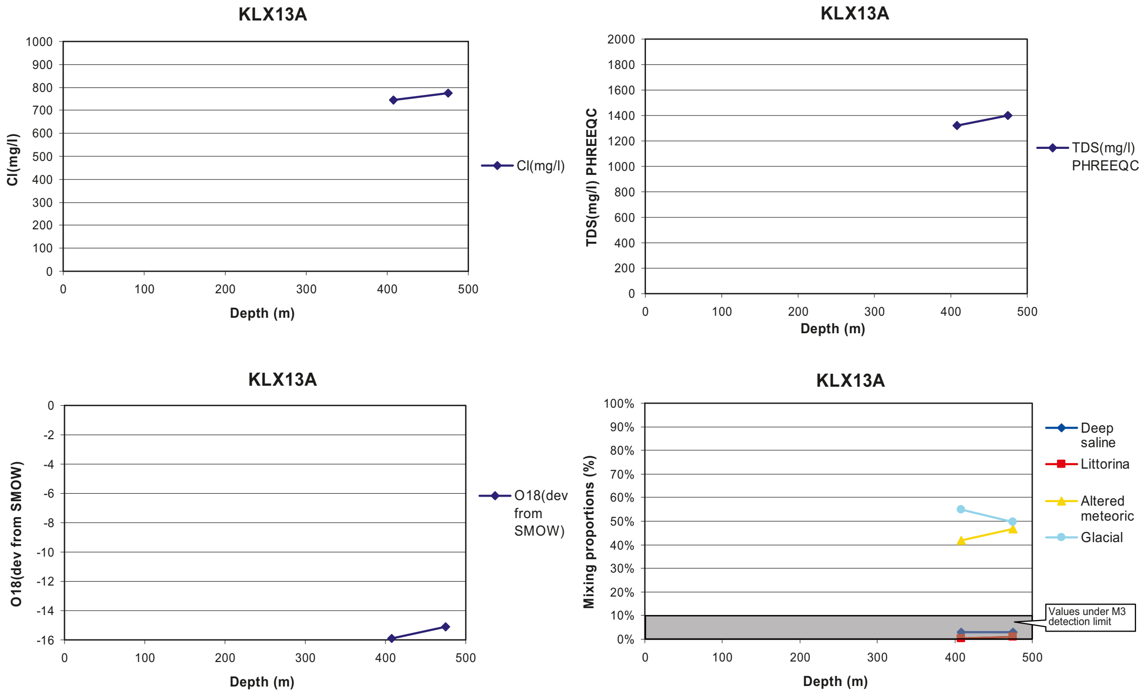


Figure 3-11. Cl, TDS, δ^{18}O, and mixing proportions along KLX13A.

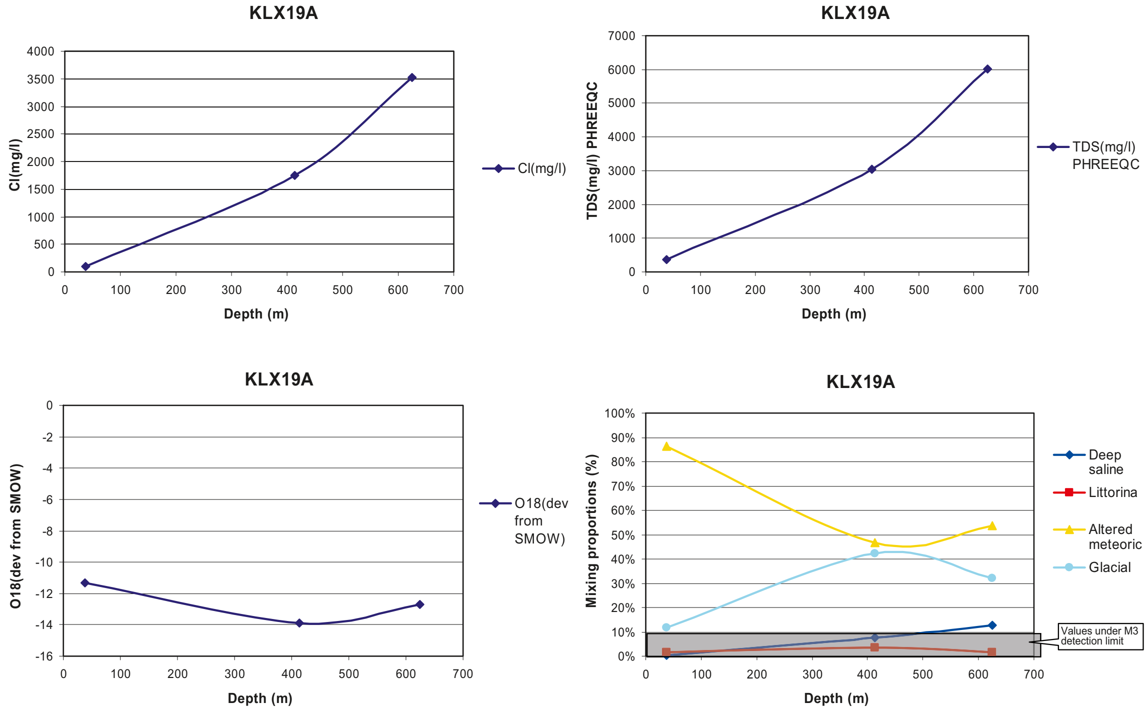


Figure 3-12. Cl, TDS, δ^{18}O, and mixing proportions along KLX19A.

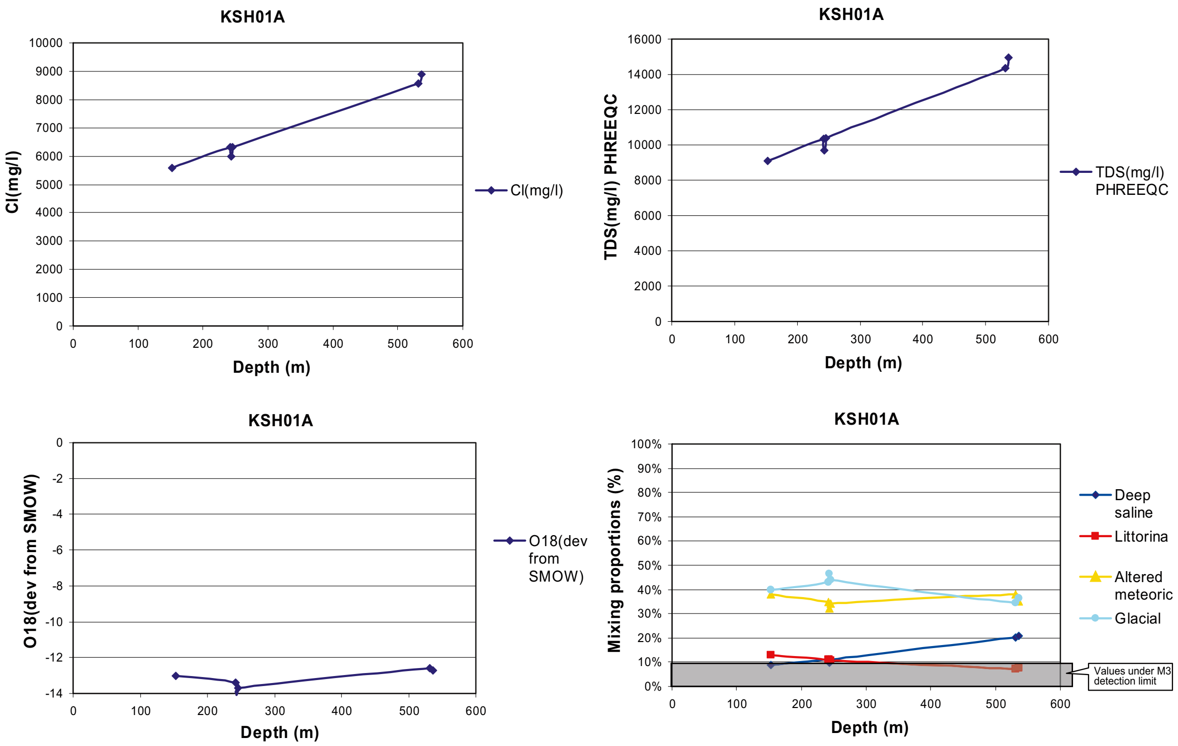


__Figure 3-13.__ Cl, TDS, $\delta^{18}O$, and mixing proportions along KSH01A.

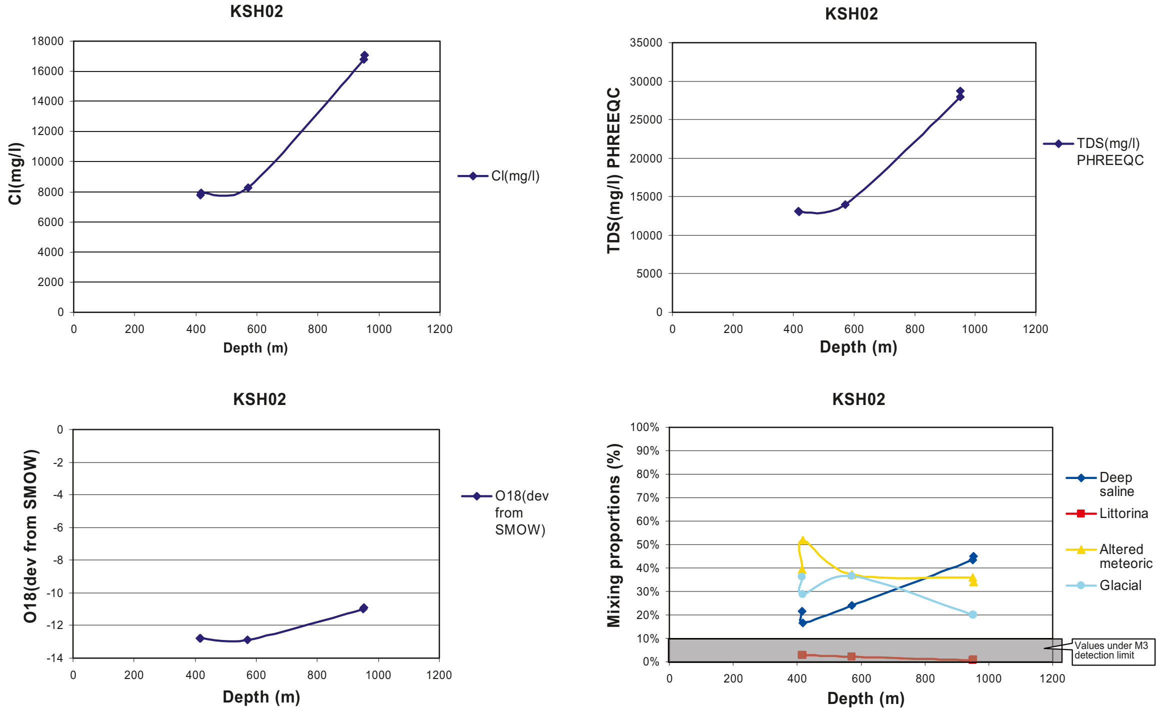


__Figure 3-14.__ Cl, TDS, $\delta^{18}O$, and mixing proportions along KSH02A.

The figures above show the measured Cl, TDS and $\delta^{18}O$ and the calculated M3 mixing proportions of SDM-Site Laxemar dataset along 14 cored boreholes, where time series were available. As a general trend, salinity (Cl) and TDS increase with depth. The lowest $\delta^{18}O$ values indicate cold recharge input. The Deep saline water component increases with depth, which is in good agreement with the Cl and TDS. The Glacial component values are highest where the lowest $\delta^{18}O$ values were measured. The Altered Meteoric mixing proportion is decreasing with depth. The Littorina Sea mixing proportions are close to or under the detection limit, meaning that Littorina Sea water is not an important component in these boreholes.

The M3 modelling gives mixing proportions along the boreholes, which, together with the Cl, $\delta^{18}O$ and TDS, can help the hydrogeologists for groundwater modelling calibration. The inclusions of samples from Laxemar 2.3 data freeze bring more understanding to the bedrock model, having more samples available at different depths. The Laxemar 2.3 model is very similar to 2.2, but more samples are included in the calculations: a total of 473 samples (from which 103 representative) for Laxemar 2.3 versus only 397 samples for Laxemar 2.2 (from which 77 representative).

3.1 Conclusions for M3 modelling of the bedrock in Laxemar 2.3

The PCA analysis presented here employs all samples with major components (Na, K, Ca, Mg, SO_4^{2-}, HCO_3^-, Cl) and isotopes the D and $\delta^{18}O$ and with the end-members Littorina, Deep saline, Glacial and altered meteoric (HLX28, 10231). The M3 modelling gives the characterisation of the SDM-Site Laxemar dataset, as follows:

a) high coverage in the M3 model, robust calculations and almost all samples are included in the PCA,

b) the use of only conservative variables does not give a unique solution, therefore the benefit of using also non conservative elements,

c) the mixing proportions including the same end-members used by the hydrogeologists are obtained (the hydrogeological models use the same end-members in their calculations),

d) the possibility of comparison with the hydrogeologists models.

The numerical values of the M3 calculations are listed in SKB's database Simon.

The M3 modelling gives mixing proportions along the boreholes, which, together with the Cl, $\delta^{18}O$ and TDS, can help the hydrogeologists in groundwater modelling calibration. The Laxemar 2.3 model is very similar to 2.2, but the existence of more samples gives the opportunity to better characterize the bedrock. This can help to obtain more mixing proportions which are then compared with the ones calculated by the hydrogeologists.

4 Uncertainty analyses and verification using the conservative elements $\delta^{18}O$ and Cl

The model used in mass balance modelling should describe as well as possible the measured data. The conservative variables Cl and $\delta^{18}O$ were used to check the accuracy of the model. These parameters are considered to be fully conservative and should not be affected by reactions; therefore the values predicted by the models should be as close as possible to the measured data. In this respect, the best model is the one which predicts the best conservative parameters, and that should not be changed by the calculations. Figures 4-1 and 4-2 show the calculated values obtained with the final model of Cl and $\delta^{18}O$ plotted against the measured values. The perfect fit line (in black) is shown in both figures.

The measured values, when compared with the predictions given by the models, should show that the best model is the one with the smallest error. The model predicts the $\delta^{18}O$ fairly well, when compared with the ideal fit line. The Cl is slightly over-predicted.

In order to quantify the accuracy of the model, the RMSE (root mean square error) was calculated for the 3 different models. The best model is the one with the smallest error, as per the following calculations:

1. Calculate the difference between data and model = the "error" on the model with respect to the data: y_data - y_model.
2. Compute the signed variance of the errors: sigma (error) and the mean error to get rid of biases.
3. Get the RMSE (Root-mean-square error) = SQRT (sigma (error) + (mean_error)^2).

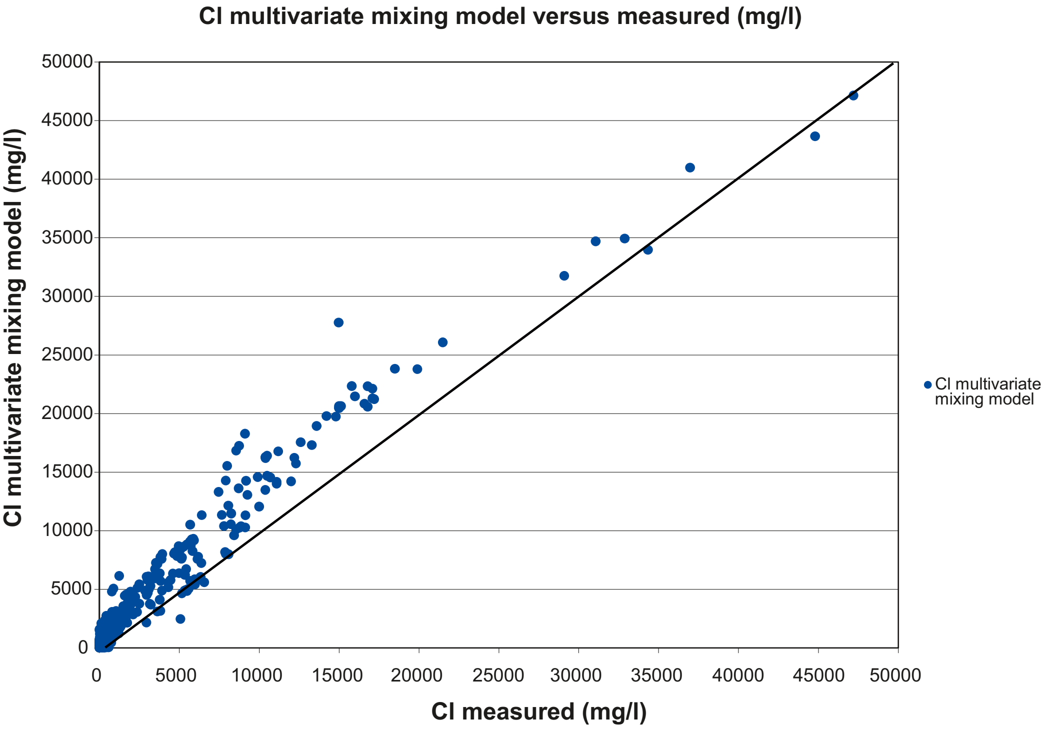


Figure 4-1. *Cl (mg/l) measured versus multivariate mixing model. The Cl is one of the variables used in the M3 calculations. The model uses all the variables (major elements and δ^2H and $\delta^{18}O$) and predicts the new values of all the parameters used. The deviation for each parameter from the measured value to the calculated value represents the effects of mixing and/or reactions. As the Cl is a conservative parameter, the calculated values should not differ from the measured values. The black line is the perfect fit line. The model over predicts Cl above the measured values of 500 mg/l.This is due to the model error. In M3 all the waters are mixed, and proportions of deep saline water type are present (even if in very small proportions) in all the samples. Therefore a small proportion of deep saline water in the shallow samples will increase significantly the calculated Cl.*

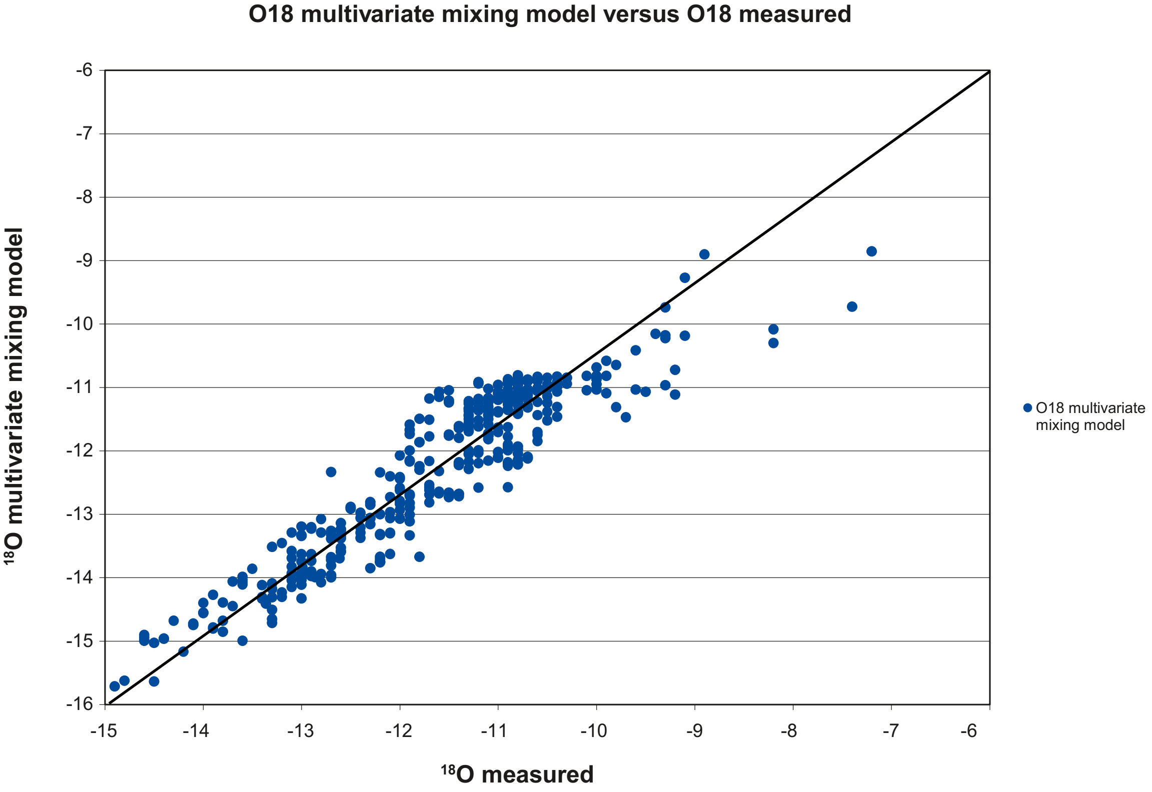


Figure 4-2. *$\delta^{18}O$ measured versus multivariate mixing model. The $\delta^{18}O$ is one of the variables used in the M3 calculations. The model uses all the variables (major elements and $\delta^{2}H$ and $\delta^{18}O$) and predicts the new values of all the parameters used. The deviation for each parameter from the measured value to the calculated value represents the effects of mixing and/or reactions. As the $\delta^{18}O$ is a conservative parameter, the calculated values should not differ from the measured values. The black line is the perfect fit line. The measurement uncertainty of $\delta^{18}O$ is 0.1 (one standard dev. from Nilsson, section #4, this report).*

The model with the smallest RMSE gives the best predictions. In Table 4-1 are presented the RMSE values obtained for the Laxemar 2.2 and 2.3 when different altered meteoric end-members were tested (HAS05 and HLX28).

The best model is the one that gives the smallest error in the calculation of the Cl and $\delta^{18}O$ versus the measured values and has the smallest RMSE. Therefore, the best is to use the one that most closely fits the conceptual model and the hydrochemical understanding. In this case HLX28 L2.3 was selected as the altered meteoric end-member.

Figure 4-3 shows the measured Cl values and the calculated Cl values with M3.

Table 4-1. RMSE for the Cl and δ18O predicted with the 3 different models.

	HAS05 L2.2		**HLX28 L2.2**		**HLX28 L2.3**	
	Cl	**O18**	**Cl**	**O18**	**Cl**	**O18**
variance	3,468,738	0.25	3,637,180	0.50	3,220,989	0.21
mean error^2	2,725,595	0.22	2,347,283	0.05	2,043,246	0.40
RMSE	2,489	0.68	2,446	0.74	2,294	0.78

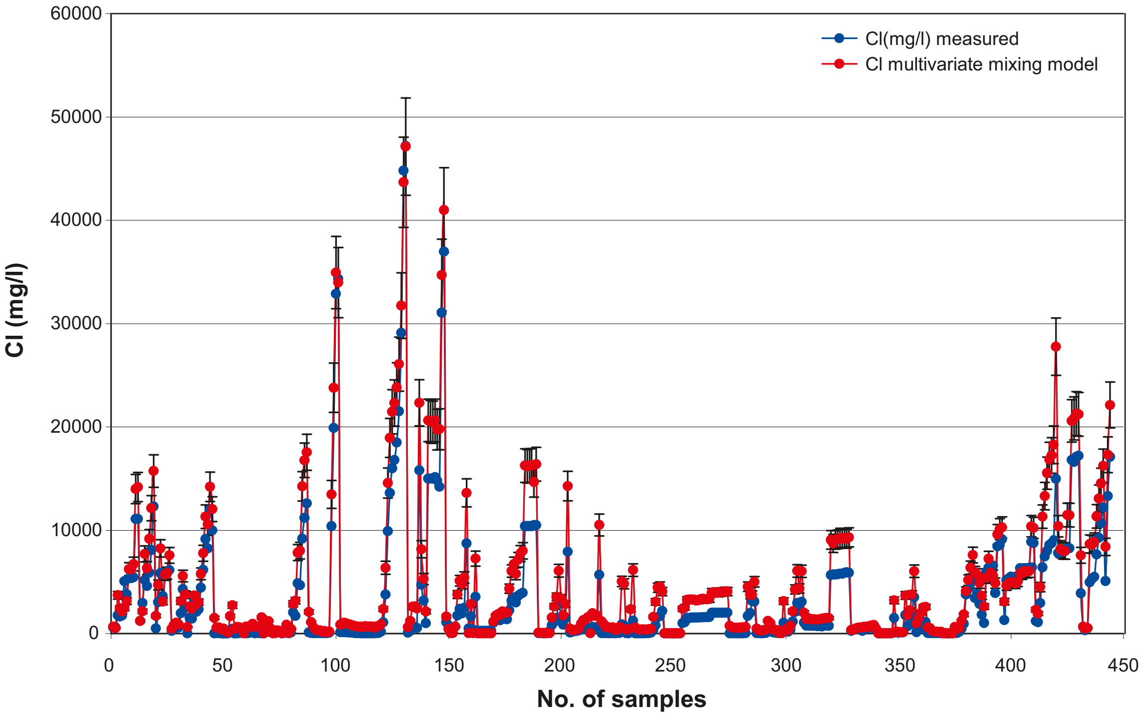


Figure 4-3. *Measured Cl mg/l content (blue dots) in samples and calculated (red dots) by applying the M3 model on groundwater data from SDM-Site Laxemar. The error bar indicates the model uncertainty in M3 (± 10%).*

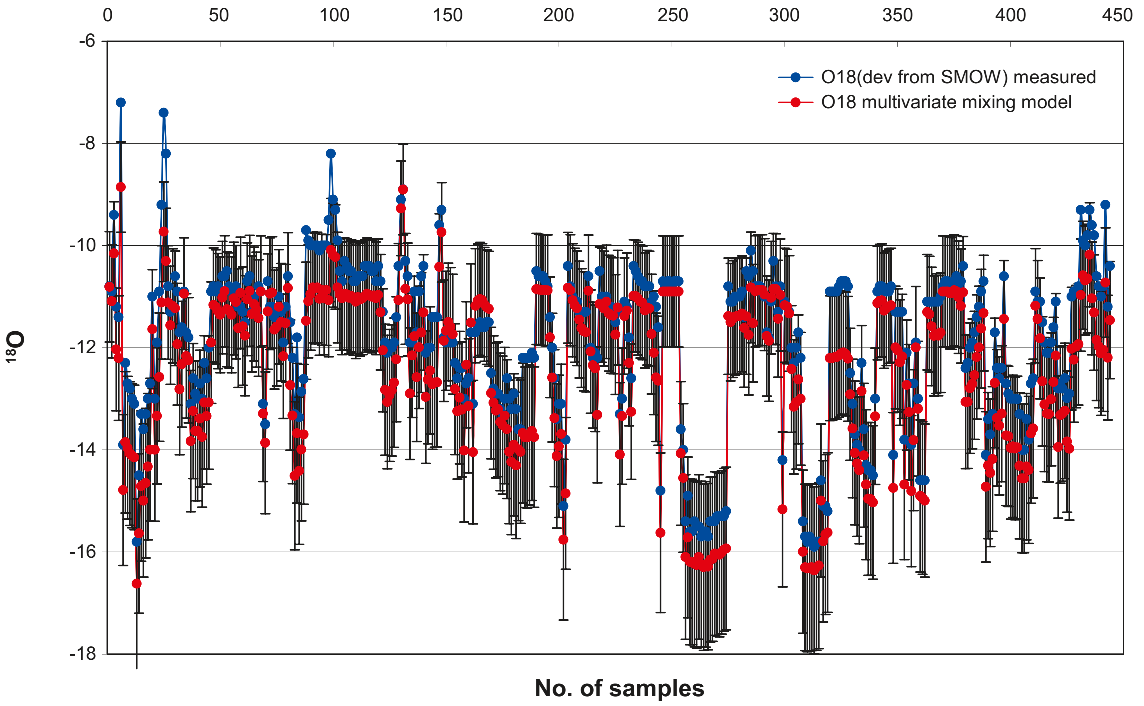


Figure 4-4. *Measured δ¹⁸O content (blue dots) in samples and calculated (red dots) by applying the M3 model on groundwater data from SDM-Site Laxemar. The error bar indicates the model uncertainty in M3 (± 10%).*

5 Site specific hydrogeochemical uncertainties

At every phase of the hydrogeochemical investigation programme – drilling, sampling, analysis, evaluation, modelling – uncertainties are introduced which have to be accounted for. They should be addressed fully and clearly documented to provide confidence in the end result, whether it will be the site descriptive model or repository safety analysis and design /Smellie et al. 2002/. The uncertainties can be conceptual uncertainties, data uncertainty, spatial variability of data, chosen scale, degree of confidence in the selected model, and error, precision, accuracy and bias in the predictions. Some of the identified uncertainties recognized during the Laxemar modelling exercise are discussed in Nilsson, section #4, this report.

The following data uncertainties have been estimated, calculated or modelled:

- Drilling; may be ± 10–70%.
- Effects from drilling during sampling; the effects from drilling are analysed more in detail in Gascoyne and Gurban, section #3 in this report.
- Sampling; may be ± 10%.
- Influence associated with the uplifting of water; may be ± 10%.
- Sample handling and preparation; may be ± 5%.
- Analytical error associated with laboratory measurements; for the elements used in M3 calculations the analytical error can be up to 13% (as per Table 2-1 in Nilsson, section # 4, this report).
- The M3 model uncertainty; is ± 0.1units within the 90% confidence interval.
- Groundwater variability (based on the Cl values) at Laxemar during groundwater sampling (first/last sample) is less than 20% for 22 sections with time series, except for the following sections:

  KLX03A (–379.85) Category 3, possible instability, borehole used later for tracer tests, variability 33.65%
  KLX03A (–700.6) Category 5, unstable, possible short-circuiting, borehole used later for tracer tests, variability 75.11%
  KLX07A (–569.69) Category 5, monitoring section, Short-circuiting, variability: 428.3%
  KLX17A (–342.32) Category 3, Instability, variability: 132.68%
  KLX12A (–501.12) Category 4
  KLX17A (–547.97) Category 5, severe short- circuiting, variability: 94.71%
  KLX19A (–413.86) Category 3, Monitoring section, variability: 150.36%

Conceptual errors can occur from e.g. the palaeohydrogeological conceptual model. The influences and occurrences of old water end-members in the bedrock can only be indicated by using certain element or isotopic signatures. This is supported by the δ^{37}Cl analyses which indicate water that may be more than 1.5 million years old. With time, it is more difficult and ambiguous to trace the origin of the groundwater. The uncertainty is therefore generally increasing with the age of the end-member. The relevance of an end-member participating in the groundwater formation can be tested by introducing alternative end-member compositions or by using hydrodynamic modelling to test if old water types can reside in the bedrock during prevailing hydrogeological conditions.

5.1 Model uncertainties

The following factors can cause uncertainties in M3 calculations:

- Input hydrochemical data errors originating from sampling errors caused by the effects from drilling, borehole activities, extensive pumping, hydraulic short-circuiting of the borehole and uplifting of water which changes the in situ pH and Eh conditions of the sample, or as analytical errors.
- Conceptual errors such as incorrect general assumptions, selecting wrong type/number of end-members and mixing samples that are not mixed. Methodological errors such as over-simplification or bias or non-linearity in the model could occur. The systematic uncertainty, which was attributable to use of the centre point to create a solution for the mixing model in the old M3 model, was solved by the M3 hyperspace model /Gómez et al. 2006/.
- Another example of a conceptual error is assuming that the groundwater composition is a good tracer for the flow system. The water composition is not necessarily a tracer of mixing directly related to flow since there is not necessarily a point source as there is when labelled water is used in a tracer test.

The uncertainties have been handled in the M3 code by calculating an uncertainty of 0.1 mixing units (with a confidence interval of 90%) and stating that a mixing portion < 10% is under the detection limit of the method /Laaksoharju et al. 1999/.

5.2 Temporal and spatial variability

Temporal and spatial variability is important in order to address how well the sampled groundwaters represent the described rock volume. The temporal variability of the groundwater can be indicated by comparing, for example, the electrical conductivity (EC) values measured shortly after drilling to the results obtained during hydrogeochemical sampling and by studying the time series and subsequent monitoring. In these particular cases, sections sampled for complete chemical characterisation (CCC) in boreholes KLX03 and KLX08A are compared with results from the resistivity logging and tube sampling.

The plots in the Figure 5-1 show the variability in the field data obtained with different types of measurement over time. This can indicate the variability of the system.

5.3 Analytical uncertainity handled by M3

As explained above, the uncertainties can be conceptual uncertainties, data uncertainty, spatial variability of data, chosen scale, degree of confidence in the selected model, and error, precision, accuracy and bias in the predictions. For example, the analytical error of the samples may be ± 10%. This possible error was tested with the M3 code. In Figure 5-2, the location of a given sample in the PCA (sample 1622 from HAS13) and the location of two synthetic samples made by adding/removing 10% from the initial composition is shown as an example of the impact of analytical uncertainty on the model output.

Another test was made for a sample nearest to the deep saline end-member. To the sample from KLX02 (sample number 2931), were added, respectively removed 10% to/from the original composition. As shown in the Figure 5-3, the spread between the sample location and the ± 10% locations, is larger than in the case of the sample 1622 from Figure 5-2. This is due to the fact that the sample is closer to the deep saline end-member, which has a very high Cl content, and therefore ± 10% represents a larger variation in the values. However, the mixing proportions calculated with the new model are within the model error (± 10%).

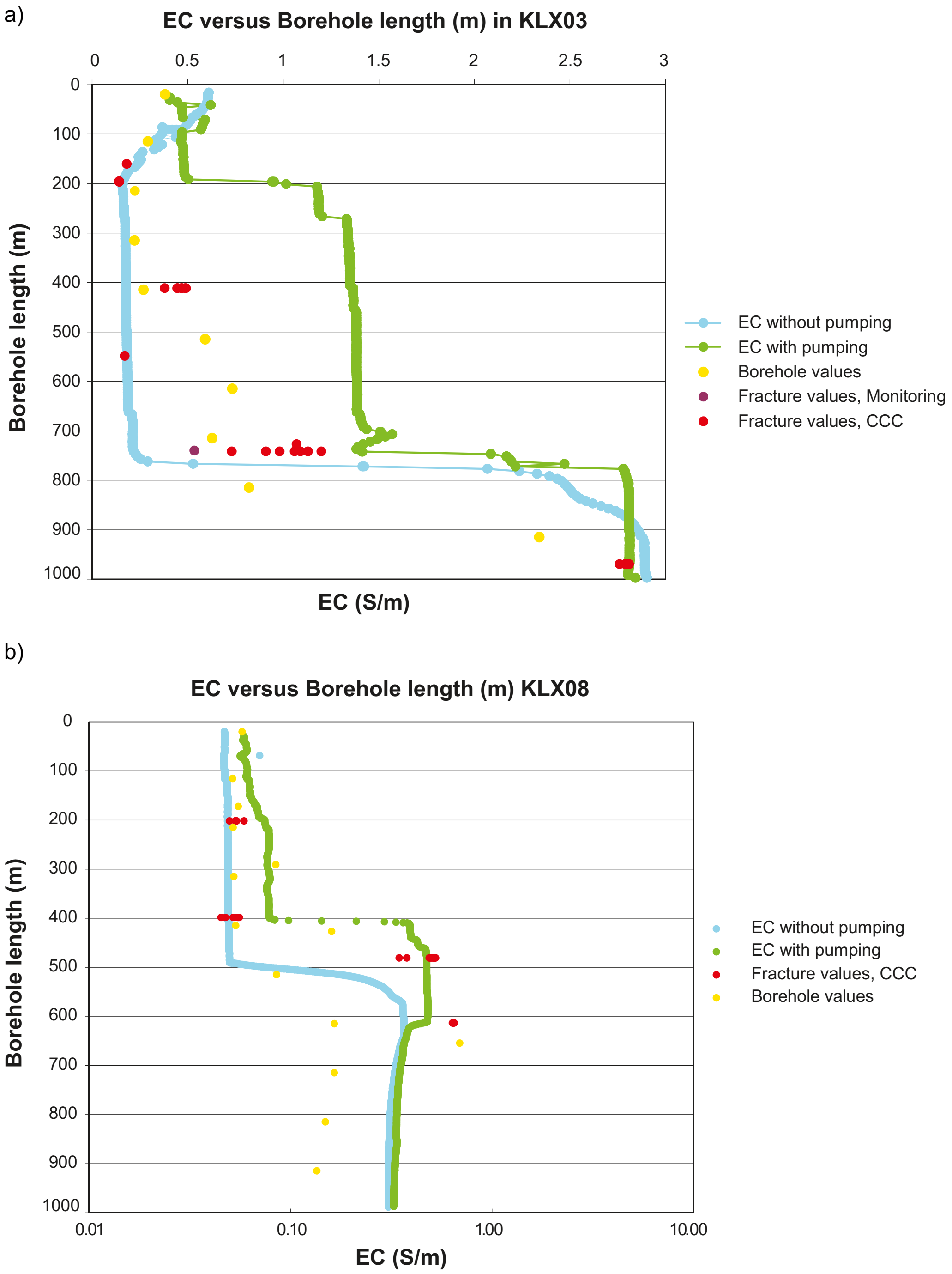


***Figure 5-1.** The electrical conductivity is measured during hydraulic logging of the freshly drilled borehole KLX03(a) and KLX08A (b) (borehole values); The borehole values are compared with the conductivity of the samples taken: 1) in the open borehole (yellow dots), and 2) with time series (red circles) taken during hydrogeochemical CCC sampling from fractures and 3) the monitoring sections (brown). The fracture groundwater samples are collected during complete chemical sampling (CCC) and during the monitoring programme.*

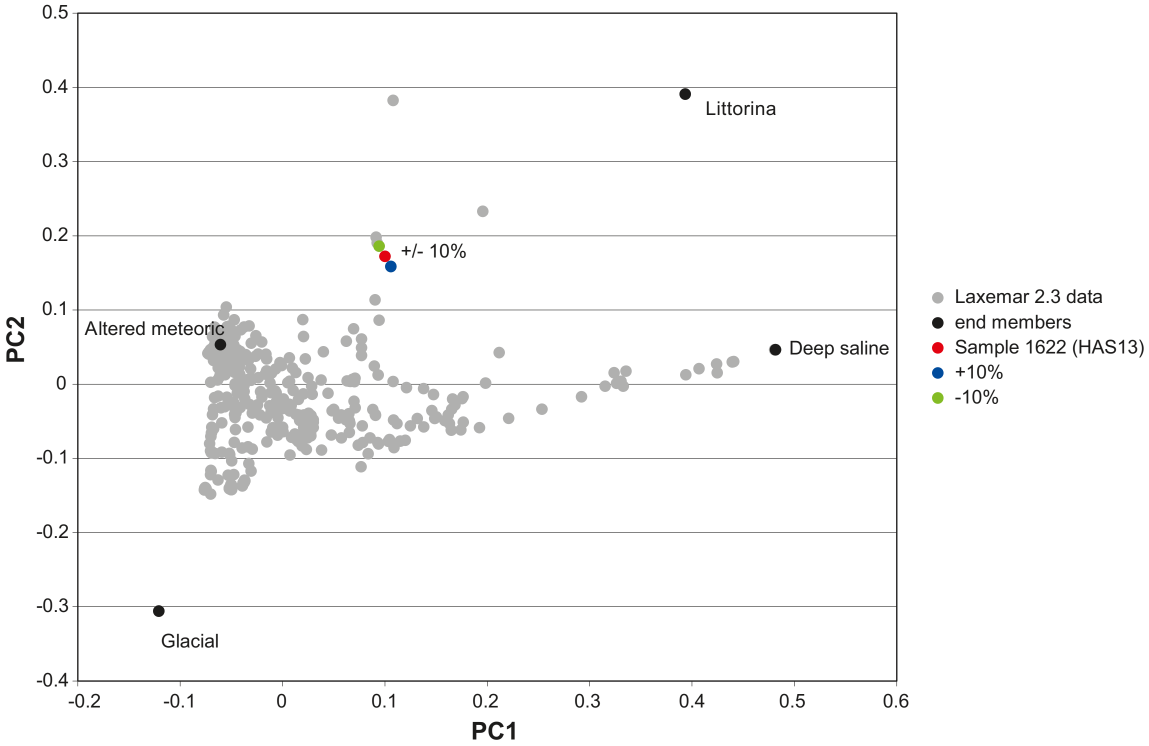


Figure 5-2. *Analytical uncertainty evaluation for Laxemar 2.3.The red dot represents sample 1622. The green and blue dots represent compositions of ± 10% from the original composition. The samples shown in the plot are all the Laxemar available samples: fracture groundwater samples (collected during complete chemical sampling (CCC) and during the monitoring programme) and borehole samples (tube sampling).*

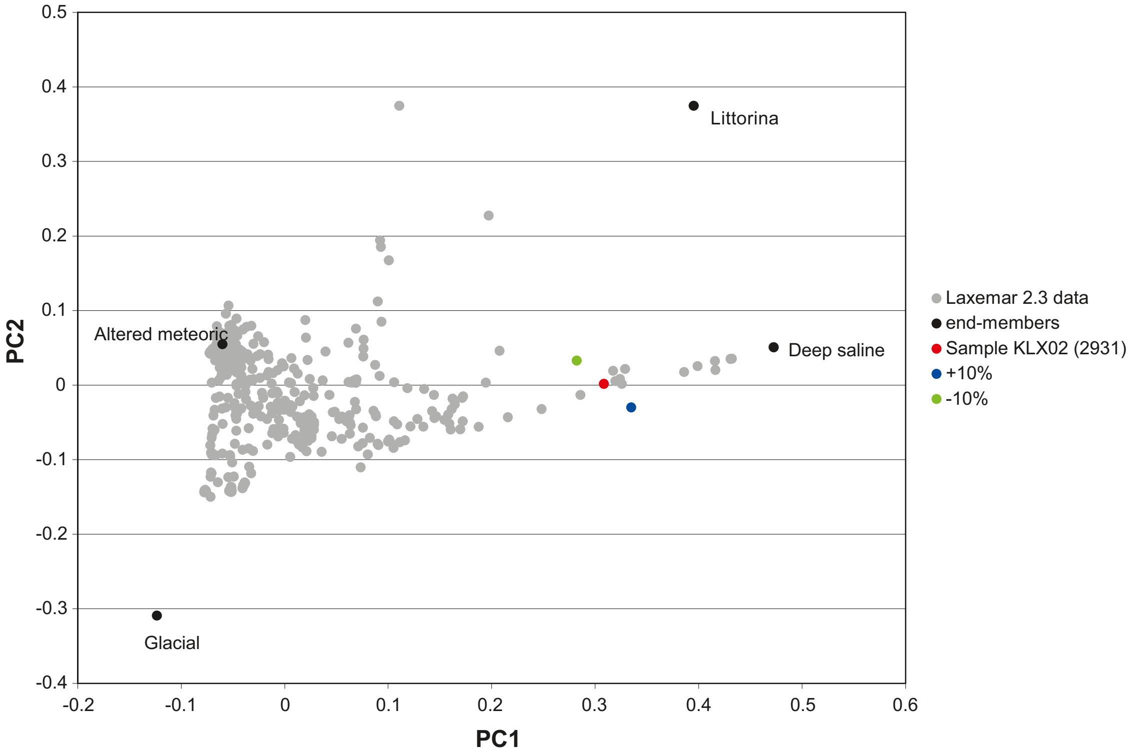


Figure 5-3. *Analytical uncertainty evaluation for Laxemar 2.3.The red dot represents sample 2931 from KLX02. The green and blue dots represent compositions of ± 10% from the original composition.*

6 Alternative model (model 2)

Several models were studied for the SDM-Site Laxemar: with different end-members and different variables. In this report, as an alternative, the model employing the following end-members is presented: Littorina, Altered meteoric, Old Meteoric-Glacial and Deep Saline. This model employs as variables the major elements, δ^2H and δ^{18}O.

The results obtained with the models presented in Figure 2-1 and 5-3 are compared in Figure 6-1. Both models employ the major elements and δ^{18}O and δ^2H as variables, but the end members are different. Model 1, called the final model, employs the Littorina, Deep saline, altered meteoric and glacial as end-members. Model 2, called the alternative model, employs the Littorina, Deep saline, altered meteoric and old meteoric-glacial as end-members. Figure 6-2 shows the mixing proportions calculated along the cored boreholes with the M3 code for models 1 and 2. Only the representative samples are shown.

By employing the Old Meteoric-Glacial reference water, more glacial water is predicted at depth and less-altered meteoric water. This is an option that can be evaluated together with the conceptual model made by "expert judgment". The deep saline and Littorina mixing proportions are unchanged when using glacial or old meteoric-glacial end-member.

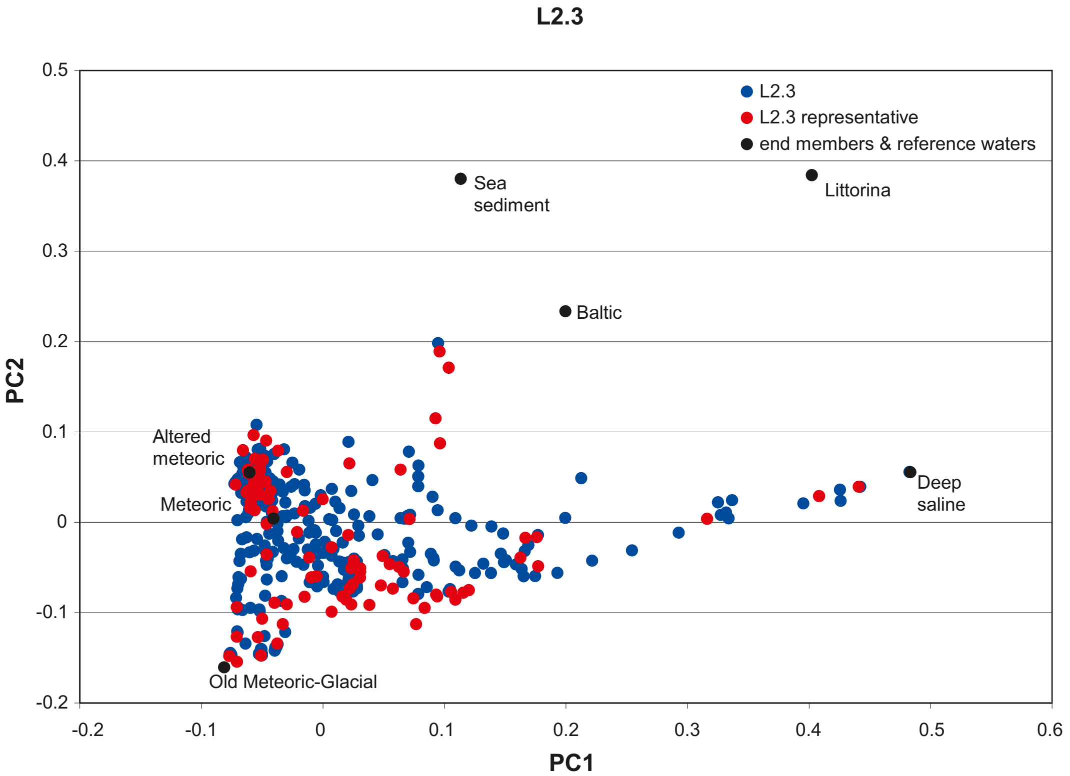
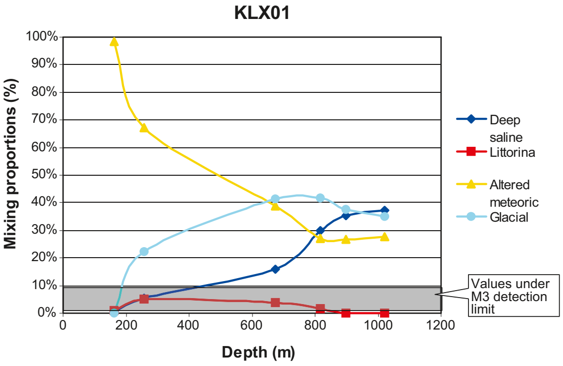
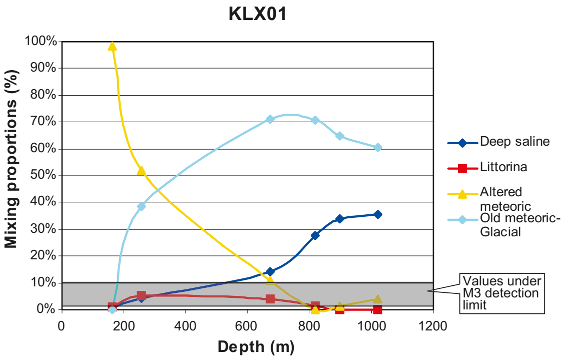


Figure 6-1. *Results of principal component analysis and identification of the reference waters for Laxemar 2.3 data set. The first principal component accounted for 0.50 of the variance, the first and second principal components 0.76, the first, second and third principal component: 0.91. The coverage is 89.4% in n-PC (as for the previous model) and 82.5% in 2D. All the major elements, $\delta^{18}O$ and δ^2H are used as variables. The Littorina, Deep Saline, Old Meteoric- Glacial and Altered Meteoric reference waters are used as end-members for the modelling. The total data available for Laxemar 2.3 are 473 samples of which 103 are considered representative (in red on the figure). The "Old Meteoric-Glacial" end-member ($\delta^2H = –118$ and $\delta^{18}O = –16$) replaces the Glacial ($\delta^2H = –158$ and $\delta^{18}O = –21$) in the M3 calculations.*


KLX01
Mixing proportions (%)
100%
90%
80%
70%
60%
50%
40%
30%
20%
10%
0%
0
200
400
600
800
1000
1200
Depth (m)
Deep saline
Littorina
Altered meteoric
Glacial
Values under M3 detection limit


KLX01
Mixing proportions (%)
100%
90%
80%
70%
60%
50%
40%
30%
20%
10%
0%
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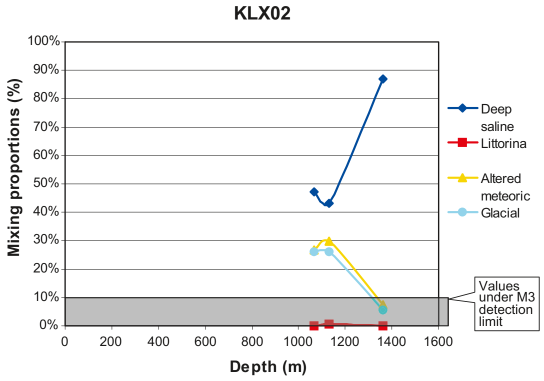
200
400
600
800
1000
1200
Depth (m)
Deep saline
Littorina
Altered meteoric
Old meteoric-Glacial
Values under M3 detection limit


KLX02
Mixing proportions (%)
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90%
80%
70%
60%
50%
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30%
20%
10%
0%
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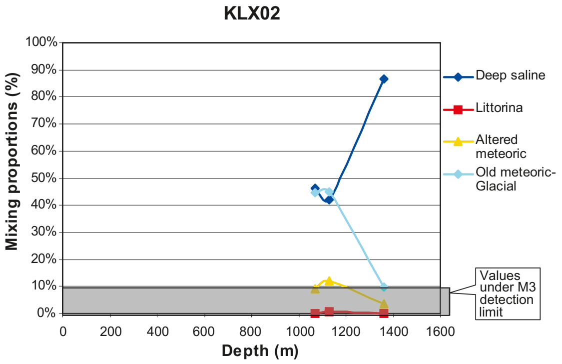
1000
1200
1400
1600
Depth (m)
Deep saline
Littorina
Altered meteoric
Glacial
Values under M3 detection limit


KLX02
Mixing proportions (%)
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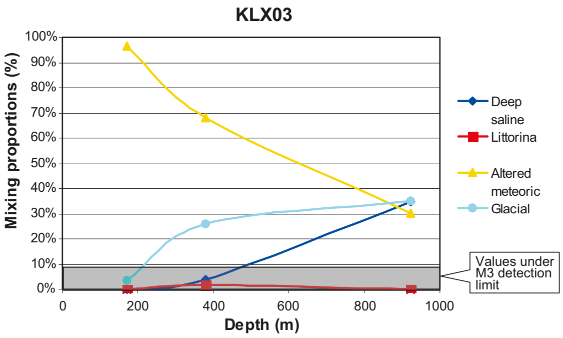
1400
1600
Depth (m)
Deep saline
Littorina
Altered meteoric
Old meteoric-Glacial
Values under M3 detection limit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Mixing proportions (%)
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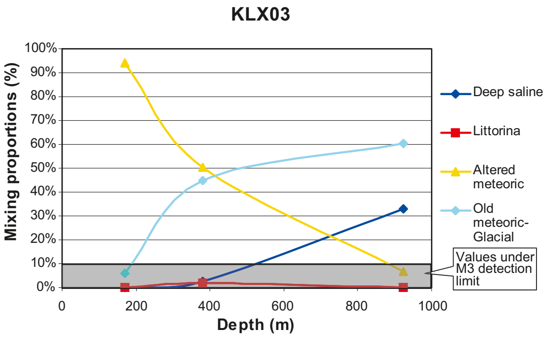
1000
Depth (m)
Deep saline
Littorina
Altered meteoric
Glacial
Values under M3 detection limit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Mixing proportions (%)
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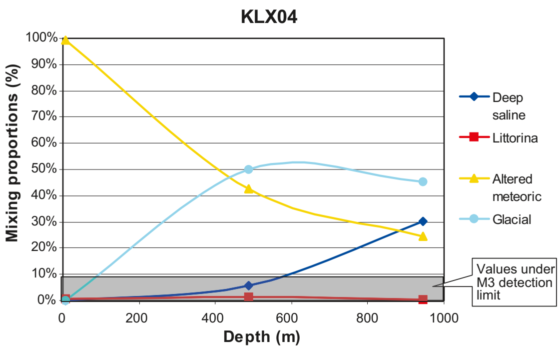
Depth (m)
Deep saline
Littorina
Altered meteoric
Old meteoric-Glacial
Values under M3 detection limit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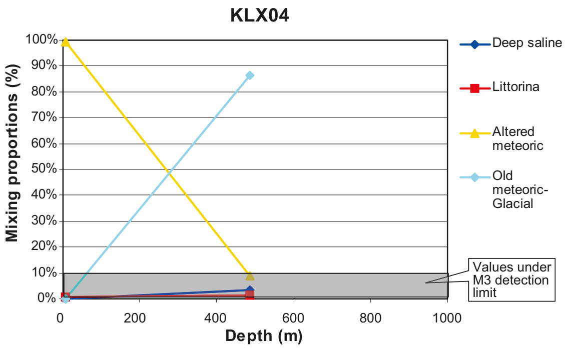
Depth (m)
Deep saline
Littorina
Altered meteoric
Glacial
Values under M3 detection limit


KLX04
Mixing proportions (%)
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90%
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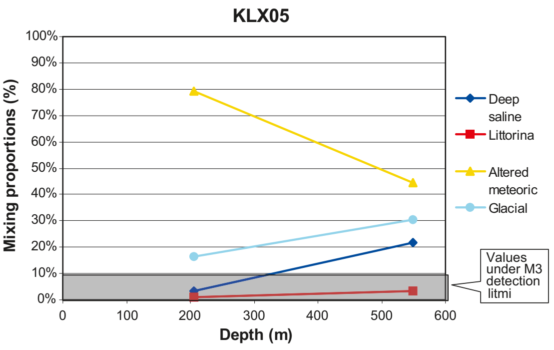
Depth (m)
Deep saline
Littorina
Altered meteoric
Old meteoric-Glacial
Values under M3 detection limit


KLX05
Mixing proportions (%)
100%
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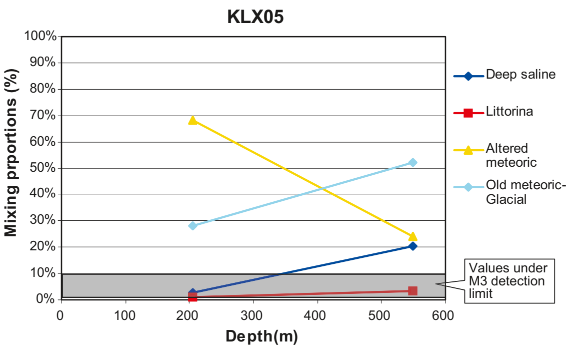
Depth (m)
Deep saline
Littorina
Altered meteoric
Glacial
Values under M3 detection litmi


KLX05
Mixing proportions (%)
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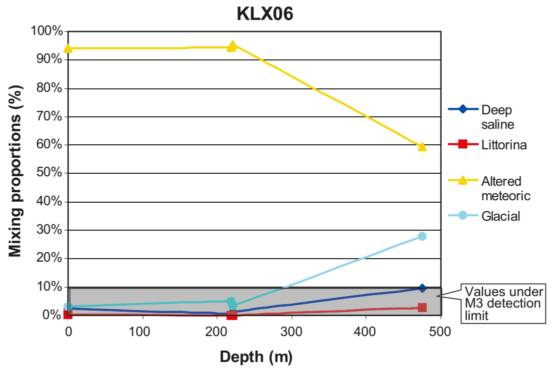
Depth(m)
Deep saline
Littorina
Altered meteoric
Old meteoric-Glacial
Values under M3 detection limit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Mixing proportions (%)
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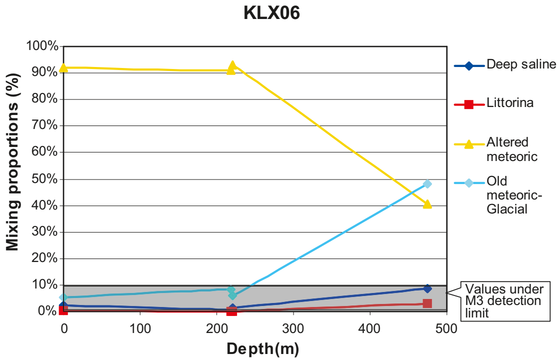
Depth (m)
Deep saline
Littorina
Altered meteoric
Glacial
Values under M3 detection limit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Mixing proportions (%)
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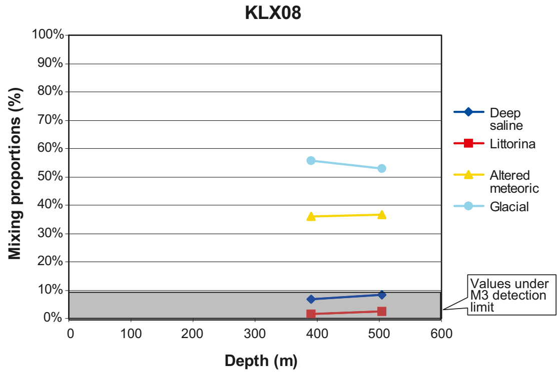
400
500
Depth(m)
Deep saline
Littorina
Altered meteoric
Old meteoric-Glacial
Values under M3 detection limit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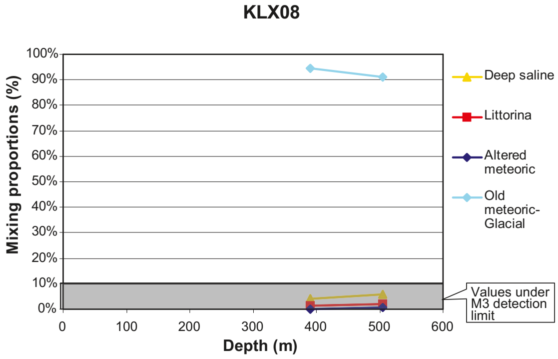
500
600
Depth (m)
Deep saline
Littorina
Altered meteoric
Glacial
Values under M3 detection limit


KLX08
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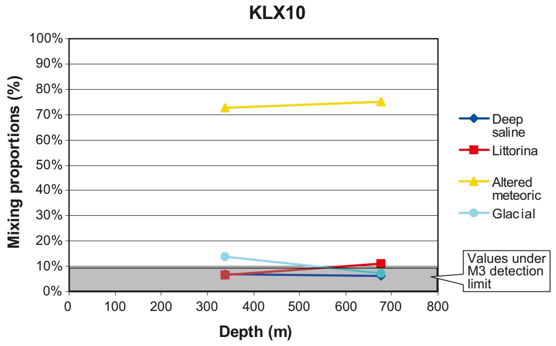
Depth (m)
Deep saline
Littorina
Altered meteoric
Old meteoric-Glacial
Values under M3 detection limit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Mixing proportions (%)
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0%
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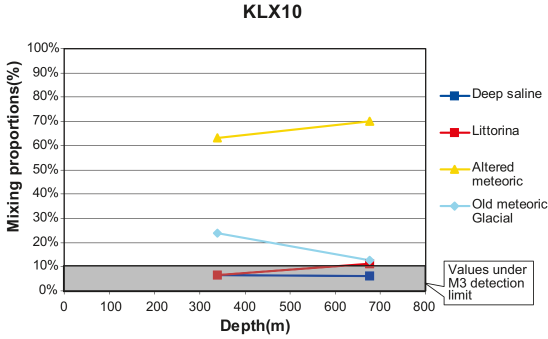
800
Depth (m)
Deep saline
Littorina
Altered meteoric
Glacial
Values under M3 detection limit


KLX10
Mixing proportions(%)
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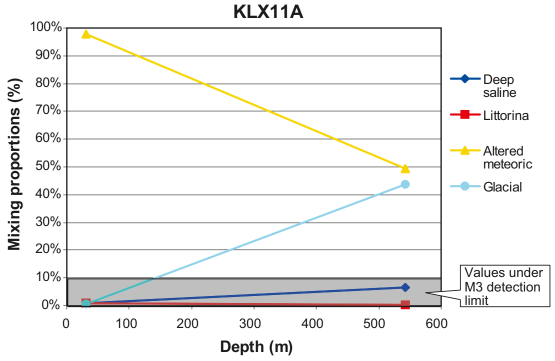
Depth(m)
Deep saline
Littorina
Altered meteoric
Old meteoric-Glacial
Values under M3 detection limit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Mixing proportions (%)
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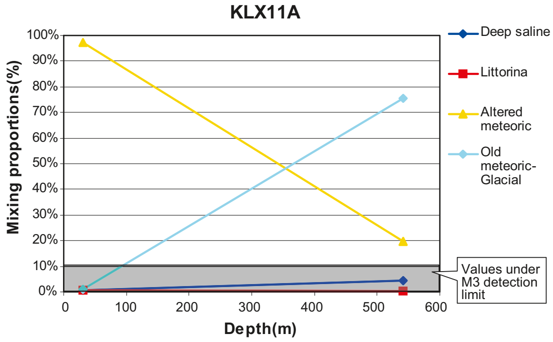
600
Depth (m)
Deep saline
Littorina
Altered meteoric
Glacial
Values under M3 detection limit


KLX11A
Mixing proportions(%)
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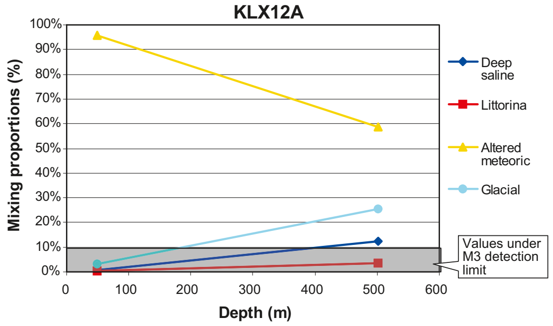
Depth(m)
Deep saline
Littorina
Altered meteoric
Old meteoric-Glacial
Values under M3 detection limit


KLX12A
Mixing proportions (%)
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80%
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10%
0%
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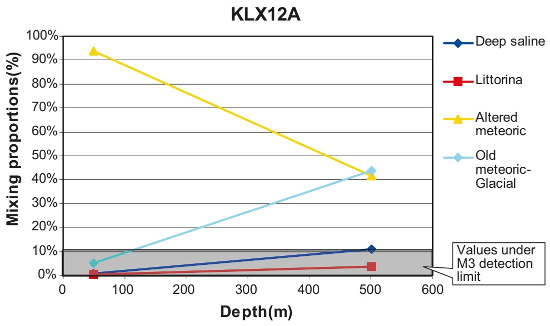
100
200
300
400
500
600
Depth (m)
Deep saline
Littorina
Altered meteoric
Glacial
Values under M3 detection limit


KLX12A
Mixing proportions(%)
100%
90%
80%
70%
60%
50%
40%
30%
20%
10%
0%
0
100
200
300
400
500
600
Depth(m)
Deep saline
Littorina
Altered meteoric
Old meteoric-Glacial
Values under M3 detection limit

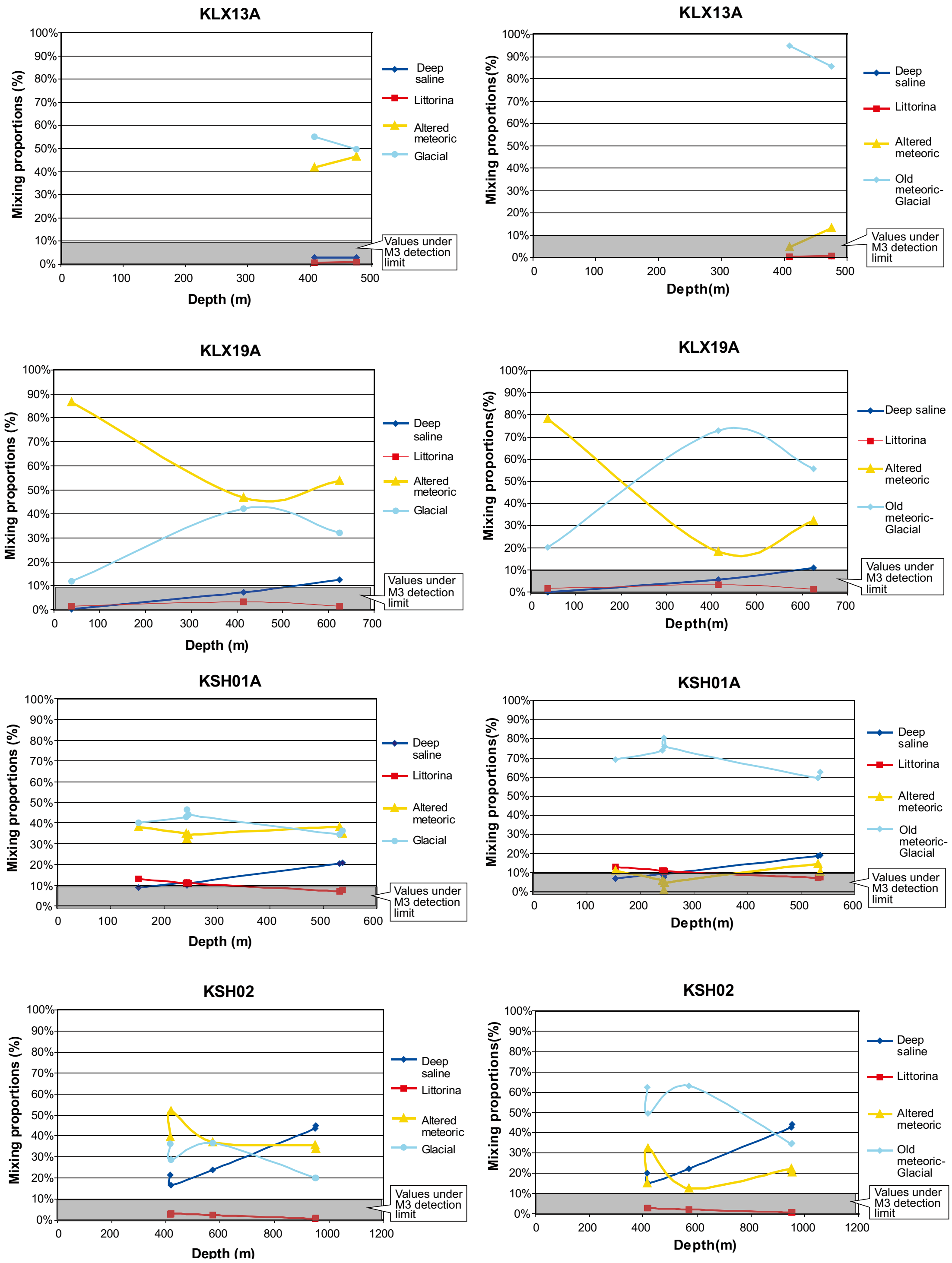


Figure 6-2. Mixing proportions along the cored boreholes with time series. Only the representative samples are presented. The left pictures represent the results obtained with model 1, where the end-members are: Littorina, deep saline, altered meteoric and glacial. The pictures on the right side represent the results obtained with model 2, where the end-members are: Littorina, deep saline, altered meteoric and old meteoric-glacial. By employing the Old Meteoric- Glacial reference water, more glacial water is predicted at depth and less-altered meteoric water. The deep saline and Littorina mixing proportions are unchanged when using glacial or old meteoric-glacial end-member.

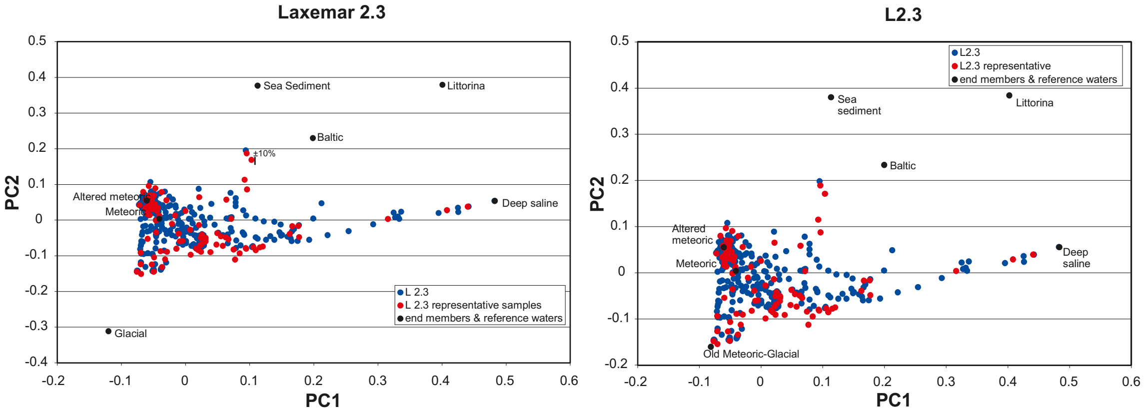


Figure 6-3. *Principal component analysis and identification of the reference waters for Laxemar 2.3 data set; left: the PCA obtained for the final model where the Glacial end-member was employed; right: the PCA obtained for the alternative model where the old meteoric- glacial end-member was employed. Both PCA show the same distribution of the samples. It is Important to note the position of the old meteoric-glacial end-member, which is much closer to the samples than the glacial end-member. This is due to the fact that its composition is closer to the hydrochemical compositions of the samples affected by the old recharge. This explains also the difference in the calculations of the mixing proportions, as shown above.*

6.1 Uncertainity analyses and verification using the conservative elements $\delta^{18}O$ and Cl for the alternative model

The best model is the one that gives the smallest error in the calculation of the Cl and $\delta^{18}O$ versus the measured values and has the smallest RMSE. Therefore, the best is to use the one that most closely fits the conceptual model and the hydrochemical understanding.

The best model is the one with the smallest error (here the model employing the old meteoric-glacial end-member), but this has to be corroborated with the conceptual model. This is an option that can be evaluated together with the conceptual model made by “expert judgment”.

The conservative variables Cl and $\delta^{18}O$ were used to check the accuracy of the model as shown in the paragraph 4 of this paper. Figures 6-4 and 6-5 show the calculated values of Cl and $\delta^{18}O$ plotted against the measured values. The perfect fit line (in black) is shown in both figures.

The Figures 4-1, 4-2, 4-3 and 4-4 are very similar to Figures 6-4 and 6-5. Both models can be used, the decision should be evaluated together with the conceptual model made by “expert judgment”. At the Laxemar site, the glacial water seems to be a major water type and therefore the Glacial end-member plays an important role. The conceptual model employs the Glacial end-member. Therefore the hydrochemical model to be used is the one employing also the Glacial end-member and called in this paper the final model.

Table 6-1. RMSE for the Cl and δ¹⁸O predicted with the final model (model1) and the alternative model (model 2).

	HLX28 L2.3 glacial end-member		HLX28 L2.3 old meteoric-glacial	
	Cl	O18	Cl	O18
variance	3,220,989	0.21	2,612,485	0.18
mean error^2	2,043,246	0.40	1,016,597	0.16
RMSE	2,294	0.78	1,905	0.58

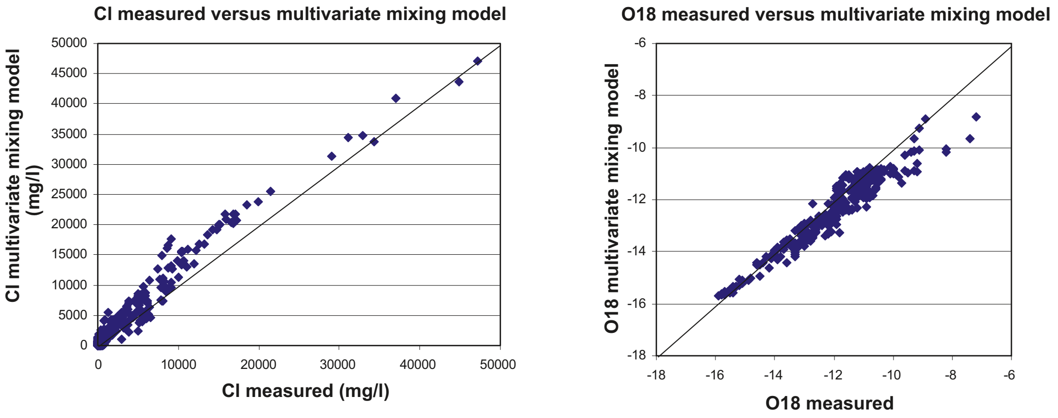


Figure 6-4. Cl and δ¹⁸O measured versus multivariate mixing model. As they are conservative parameters, the calculated values should not differ from the measured values. In black the perfect fit line. The Cl and δ¹⁸O show the same trend as in the Figures 16 and 17. Small proportion of deep saline water in the shallow samples can increase the calculated Cl. The measurement uncertainty of δ¹⁸O is 0.1 (one standard dev. from AC Nilsson, section #4 this report).

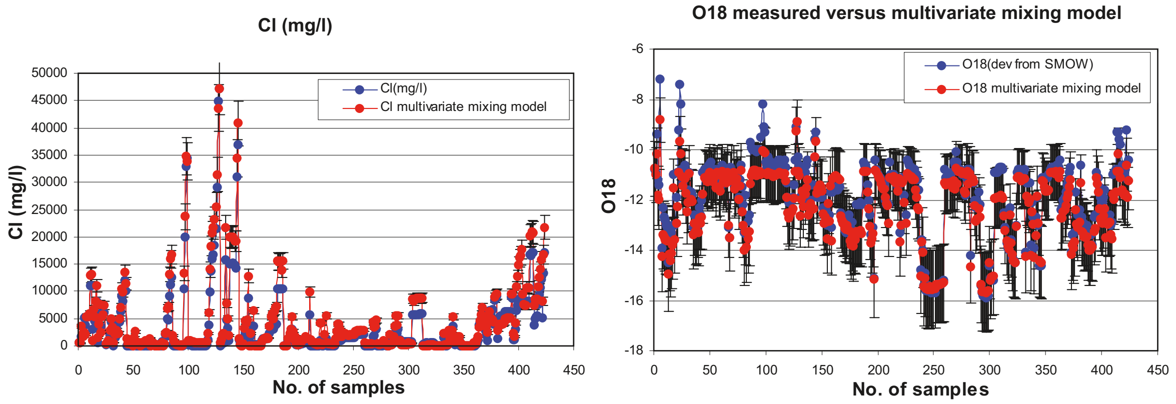


Figure 6-5. Measured Cl δ¹⁸O content (blue dots) in samples and calculated (red dots) by applying the M3 model on groundwater data from Laxemar site. The error bar indicates the model uncertainty in M3 (± 10%).

7 Concluding remarks

This work resents the SDM-Site Laxemar hydrochemical evaluation and modelling of the Laxemar data. This comprises M3 modelling, alternative models, explorative data tests and 2D visualisation of the data along the boreholes. The following conclusions are drawn:

- M3 modelling helped to summarize and understand the data, by using as variables the major elements and the isotopes $\delta^{18}O$ and D.
- Previous alternative models and the experience from Simpevarp 1.2 and then Laxemar 2.1 and Laxemar 2.2 (see Appendix 1), helped to clarify different previously unsolved issues such as: the use of variables, tests with different end-members and the use of only groundwater data in order to explain the Laxemar bedrock domain.
- The alternative models helped to address different issues such as tests with different end-members.
- The visualisation of the mixing proportions along the boreholes helps to understand the distribution of the data in SDM-Site Laxemar bedrock and to check and compare the results of different models; and therefore to choose the model which best describes the measured data.
- The different M3 modelling tests resulted in the following conclusions: a) when calculating mixing proportions only samples from the boreholes will be used, b) the meteoric end member which best describes the more shallow groundwater compositions is defined by HLX28 (10231); the other end-members such as Littorina and Glacial employed the existing modelled compositions. The use of the Littorina, Glacial and Deep saline end-members makes possible the comparison of different sites such as Laxemar and Forsmark. By employing the Old Meteoric- Glacial reference water, more glacial water is predicted at depth and less-altered meteoric water.
- From all the models tested, the one that best fits the conceptual model and the hydrogeochemical understanding was presented. As at Laxemar the glacial water seems to be a major water type, the glacial end-member plays an important role and is used in the final model.
- All the data used in the M3 modelling and the results of the modelling and visualisation along the boreholes are stored in SKB's database Simon.

8 References

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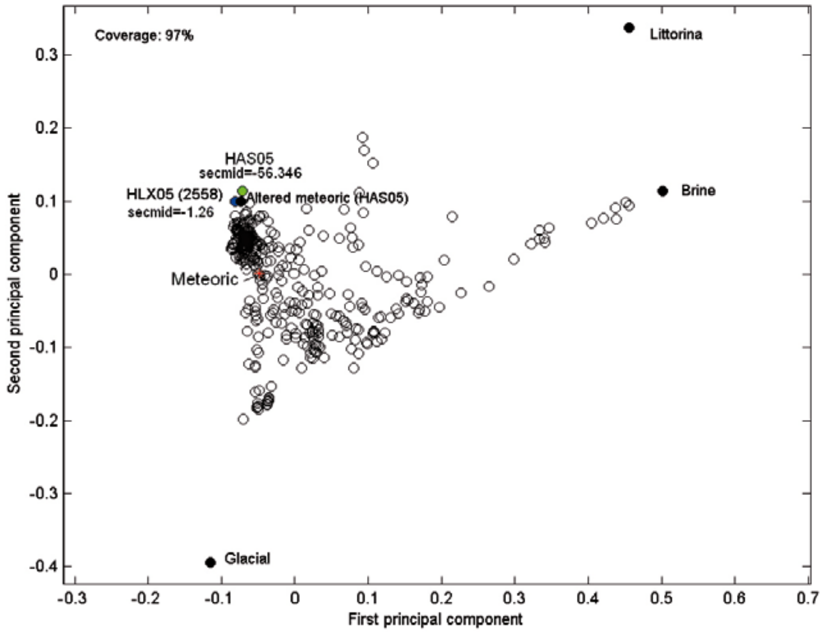
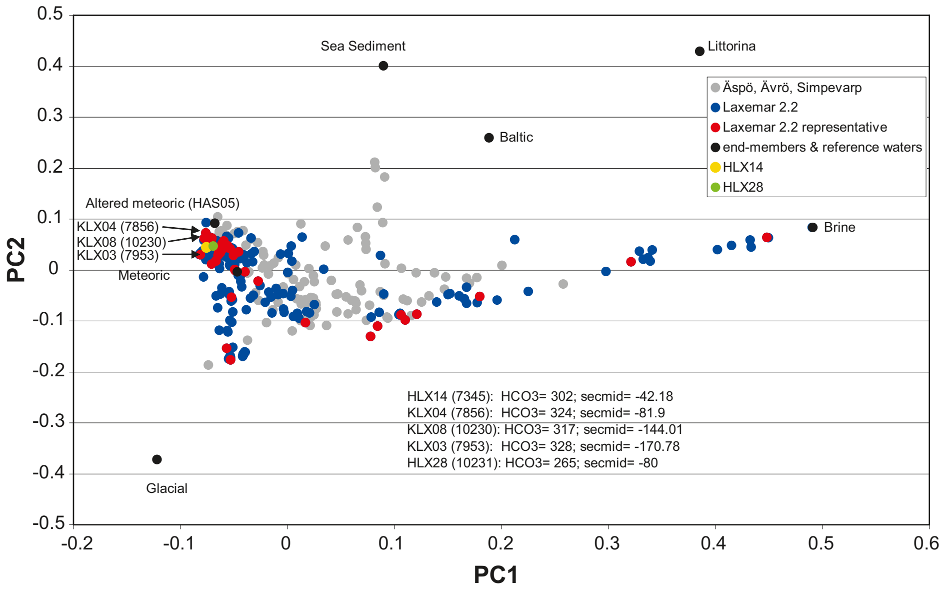
Laxemar 2.2 tests

PCA Laxemar 2.2



PCA obtained of Laxemar 2.2 dataset; the end-members are Littorina, Brine (deep saline), Glacial and Altered meteoric (HAS05). Laxemar 2.2: 397 samples with major elements, D and δ^{18}O, from which 77 representative.

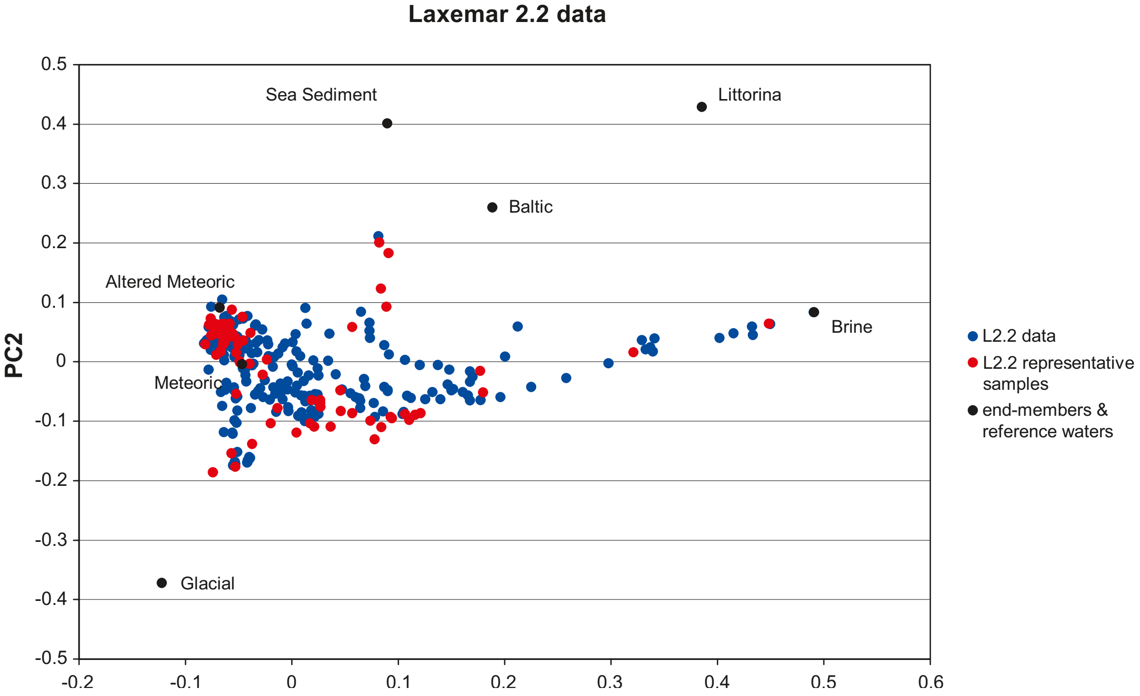
M3: coverage = 97% (387 samples); Variance: 50%, 75% and 91%.



PCA obtained of Laxemar 2.2 dataset; the end-members are Littorina, Brine (deep saline), Glacial and Altered meteoric (HAS05). In red are represented the representative samples and in blue all the other samples. Different options for the shallow end member are tested: HLX14 (7345), KLX04(7856), KLX08(10230), KLX03 (7953) and HLX28 (10231).

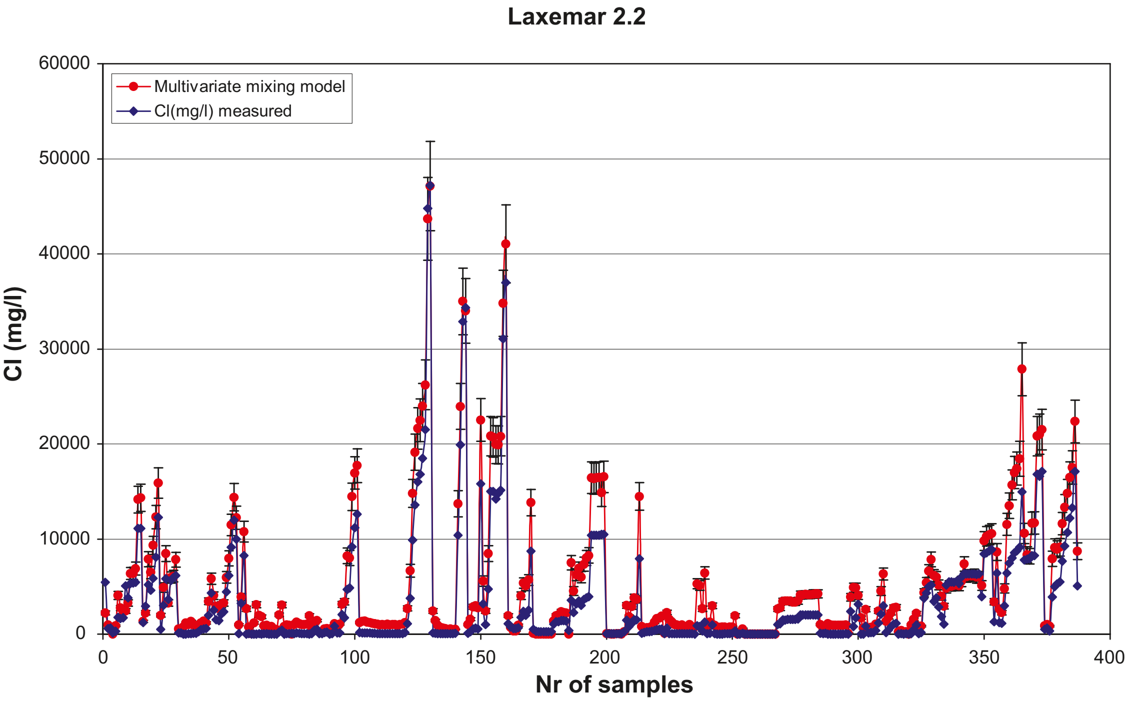
End-members used in M3 modelling of Laxemar 2.2 and Forsmark 2.2 datasets.

End Member	**ID Code**	**Cl (mg/l)**	**Na (mg/l)**	**K (mg/l)**	**Ca (mg/l)**	**Mg (mg/l)**	**HCO3 (mg/l)**	**SO4 (mg/l)**	**d2H‰**	**d18O‰**
Brine	Laxemar SGKLX02	47,200	8,200	45.5	19,300	2.12	14.1	906 (10 for F2.2)	–44.9	–8.9
Glacial		0.5	0.17	0.4	0.18	0.1	0.12	0.5	–158.0	–21
Littorina Sea		6,500	3,674	134	151	448	92.5	890	–37.8	–4.7
Altered meteoric L2.2	HAS05 (–56.346 m)	119	237	4	25	6	370	118	–73.8	–9.9
Altered meteoric L2.2	HLX28 (–80 m)	23	110	2.97	11.2	3.6	265	35.8	–76.5	–10.9
Dilute Granitic GW F2.2	HFM09 (8335) (–25 m)	181	274.0	5.60	41.1	7.5	466.00	85.10	–80.6	–11.1

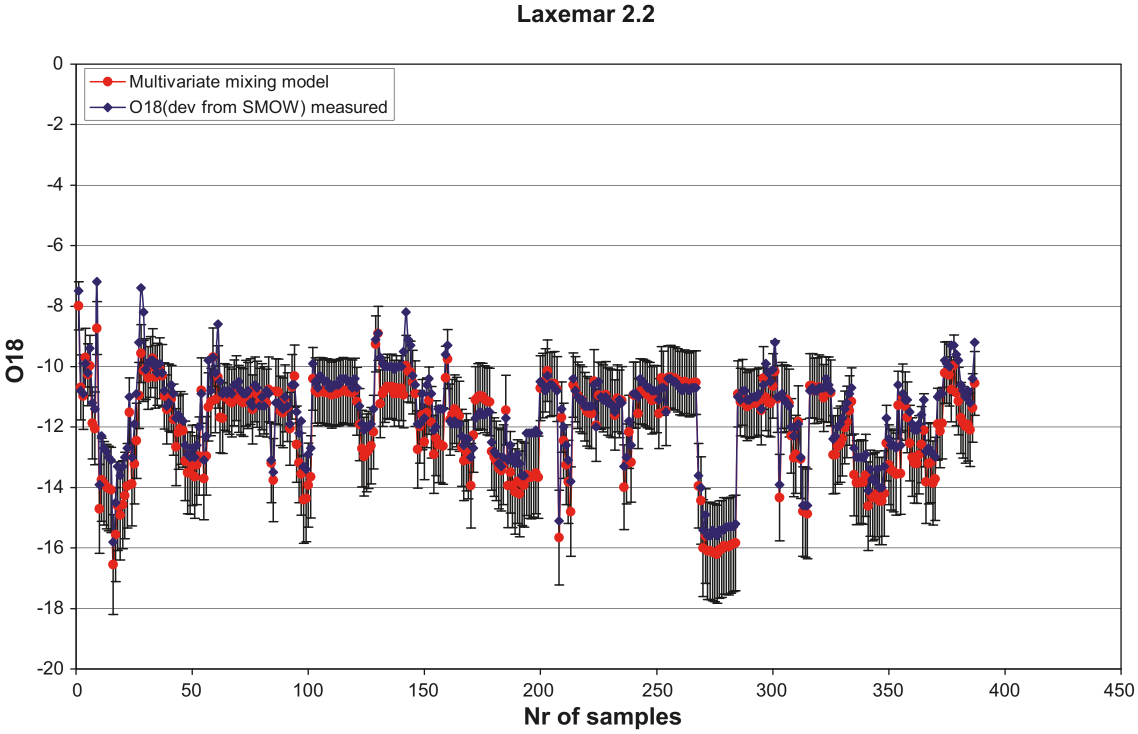


Laxemar 2.2: 397 samples with major elements, D and $\delta^{18}O$**,** from which 77 representative. M3: coverage = 97% (387 samples); Variance: 50%, 75% and 91%. The representative samples (marked in orange and green in the table) are shown in red in the plot. The end-members are: Altered meteoric (HAS05), Littorina, Brine and Glacial

Uncertainty analyses and verification using the conservative elements δ18O and Cl; results from the model where HAS05 was used as altered meteoric end member.



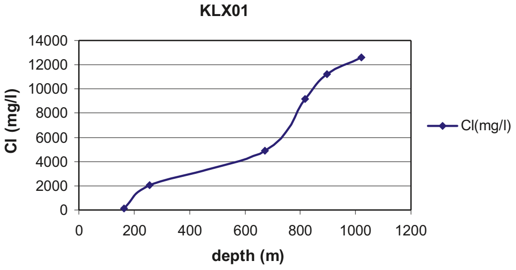
Measured Cl mg/l content (blue dots) in samples and calculated (red dots) by applying the M3 model on groundwater data from Laxemar 2.2 data. The error bar indicates the model uncertainty in M3 (± 10%).

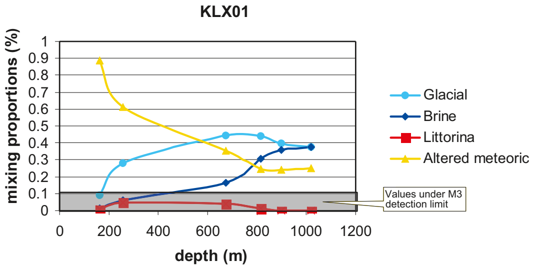


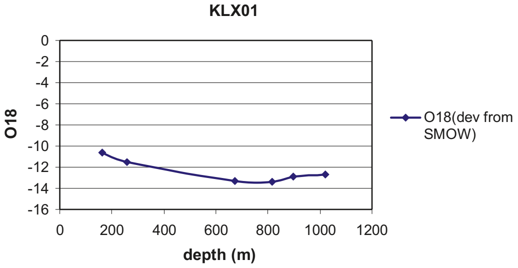
Measured δ18O (blue dots) in samples and calculated (red dots) by applying the M3 model on groundwater data from Laxemar 2.2 data. The error bar indicates the model uncertainty in M3 (± 10%).

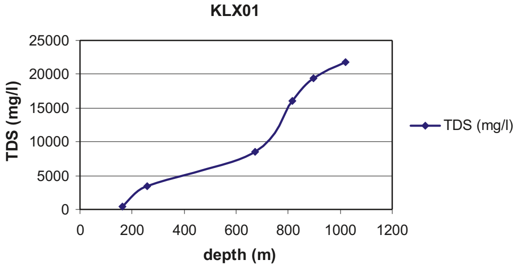
2D visualisation of the Cl, δ^{18}O, TDS and mixing proportions of the cored boreholes, obtained with the following end-members: Littorina, Glacial, Brine (deep saline) and altered meteoric (HAS05).

KLX01

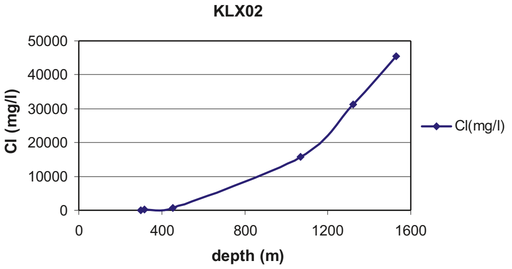


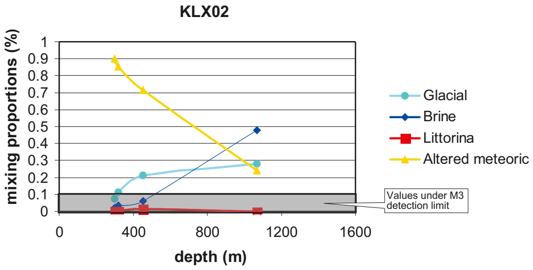


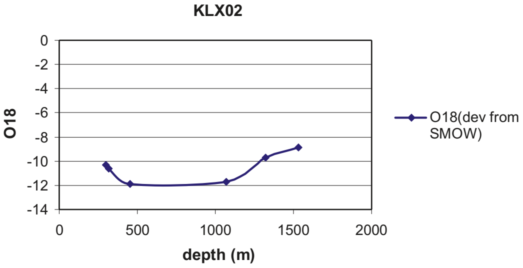


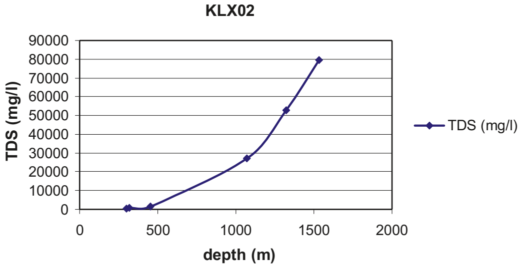


KLX02

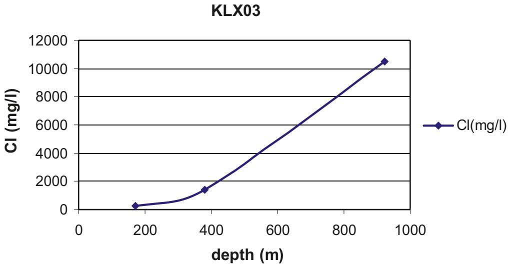


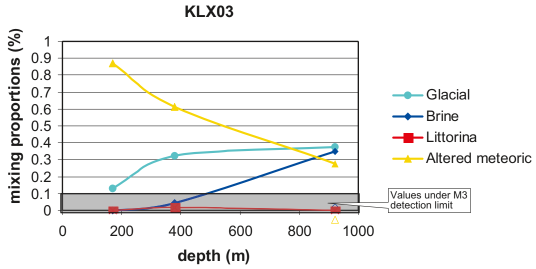


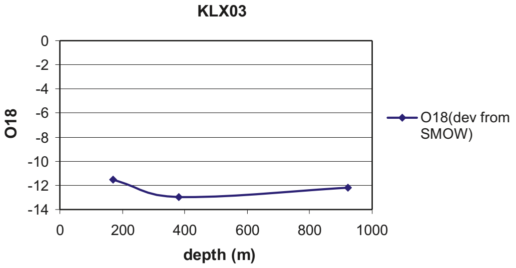


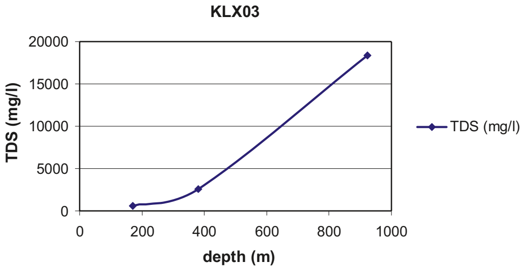


KLX03

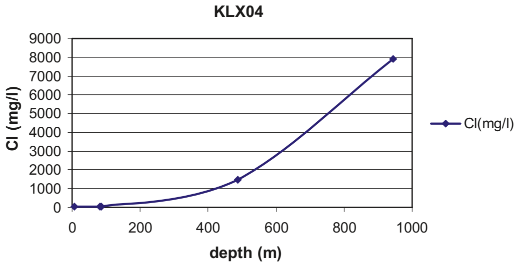


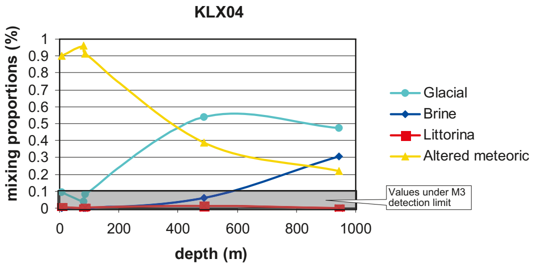


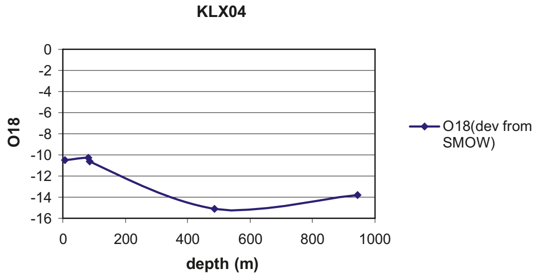


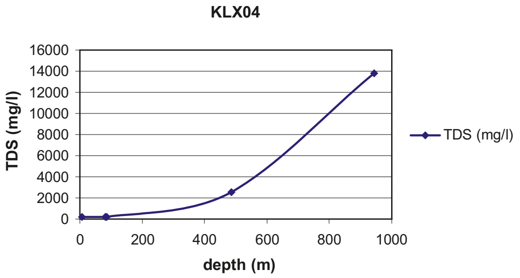


KLX04

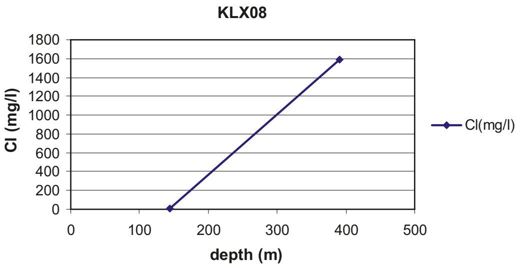


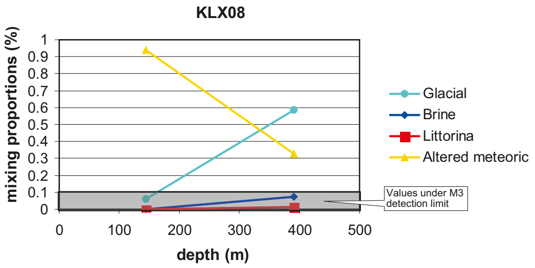


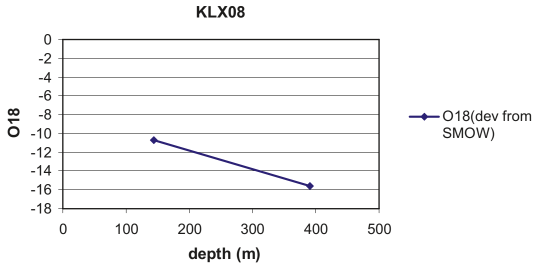


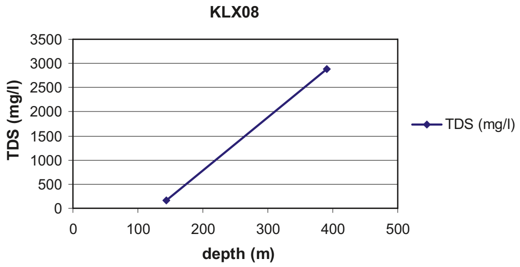


KLX08

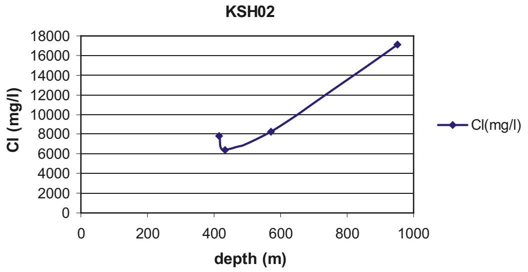


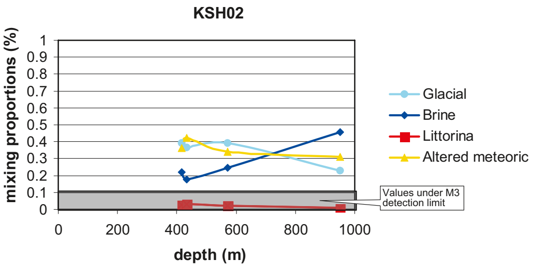


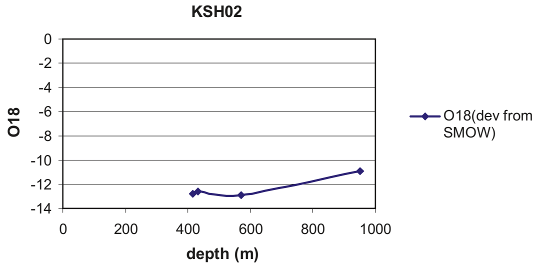


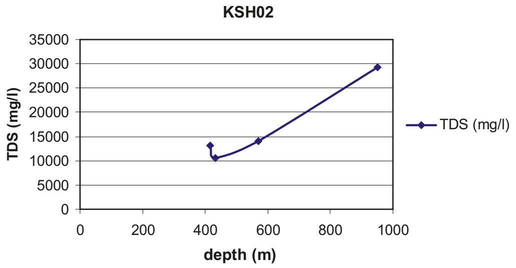


KSH02

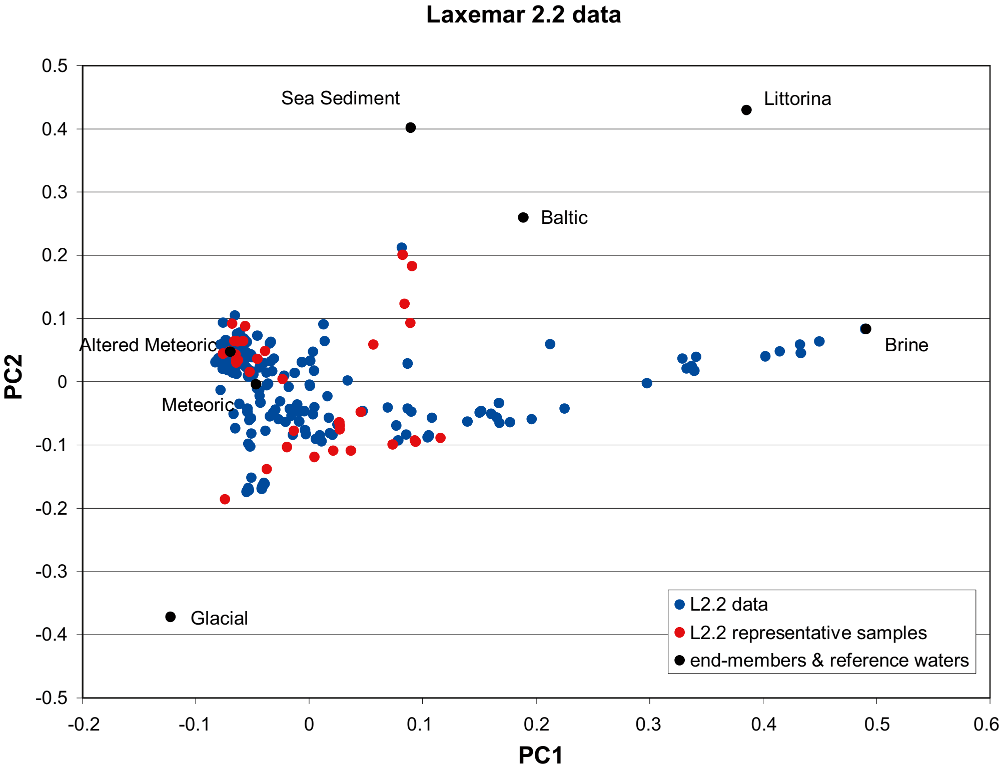






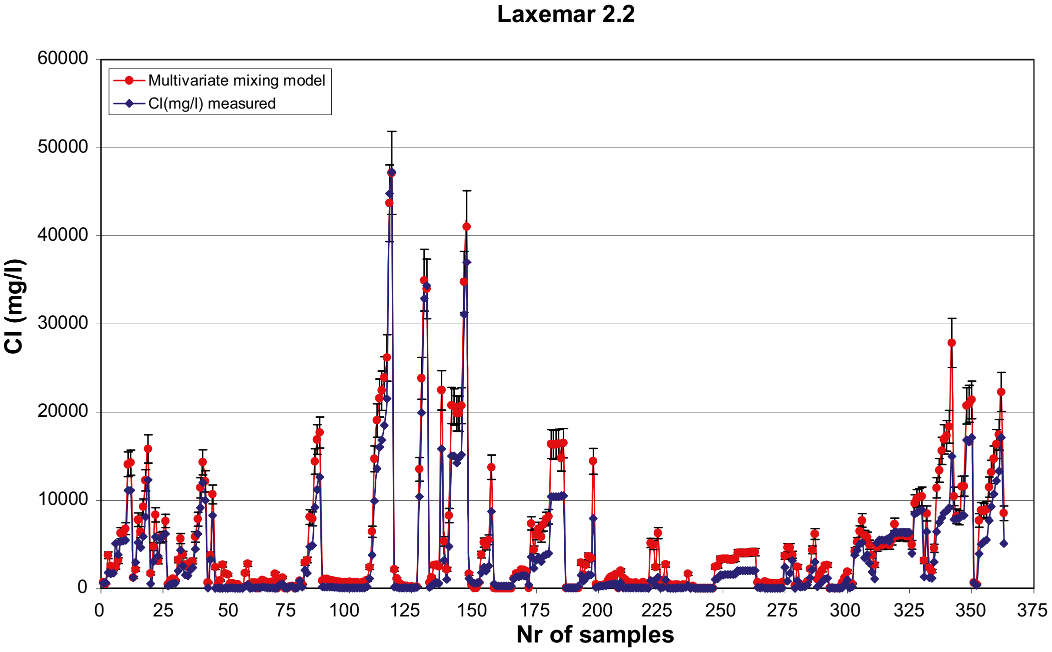


PCA obtained of Laxemar 2.2 dataset; the end-members are Littorina, Brine (deep saline), Glacial and Altered meteoric (HLX28). In red are represented the representative samples and in blue all the other samples.

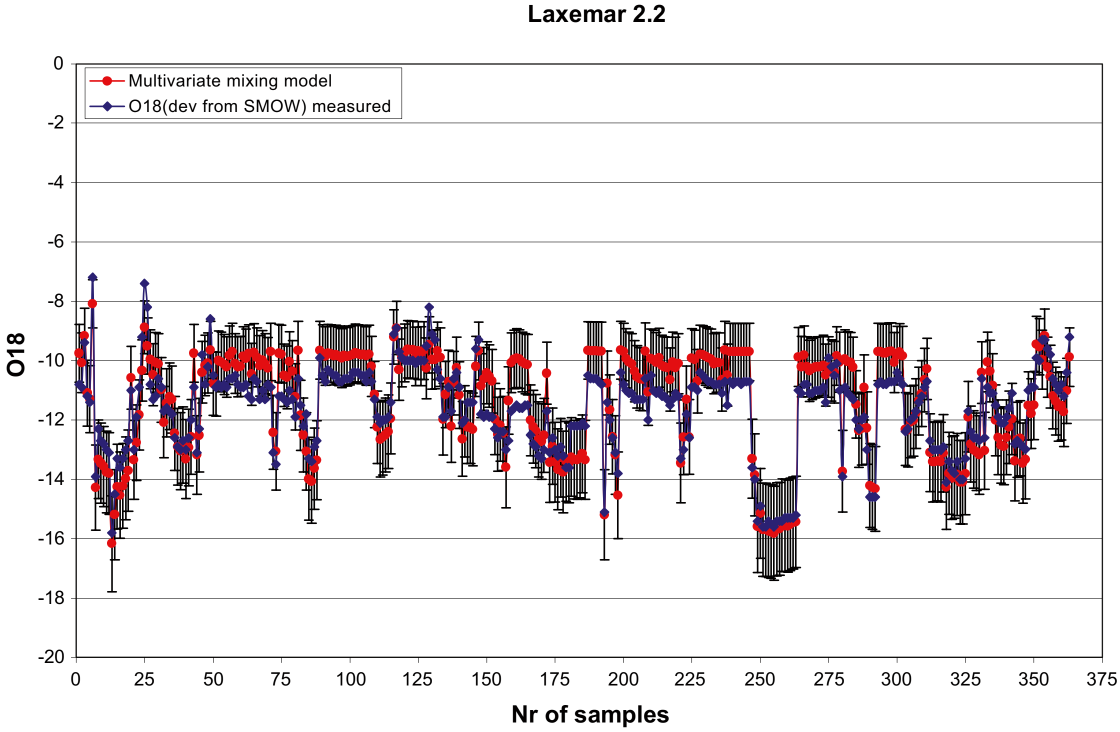


Laxemar 2.2: 397 samples with major elements, D and δ^{18}O, from which 77 representative. M3: coverage = 97% (363 samples); Variance: 50%, 75% and 91%. The representative samples are shown in red in the plot. The end-members are: Altered meteoric (HLX28/10231), Littorina, Brine and Glacial.

Uncertainty analyses and verification using the conservative elements δ^{18}O and Cl; results from the model where HLX28 was used as altered meteoric end member.



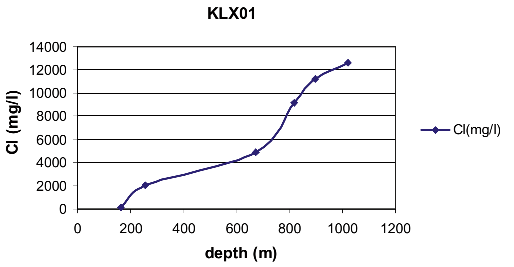
Measured Cl mg/l content (blue dots) in samples and calculated (red dots) by applying the M3 model on groundwater data from Laxemar 2.2 data. The error bar indicates the model uncertainty in M3 (± 10%). Altered meteoric end member is HLX28 (10231).

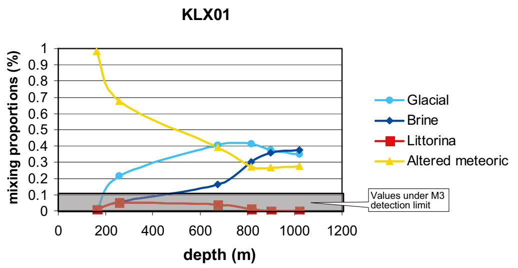


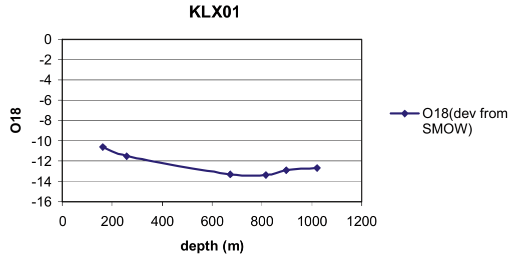
Measured δ^{18}O (blue dots) in samples and calculated (red dots) by applying the M3 model on groundwater data from Laxemar 2.2 data. The error bar indicates the model uncertainty in M3 (± 10%). Altered meteoric end member is HLX28 (10231).

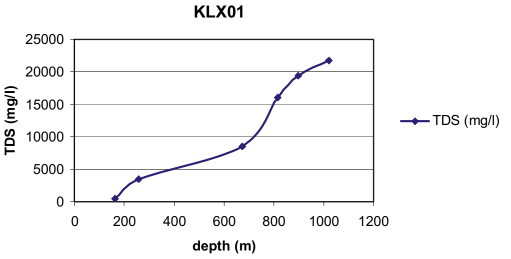
2D visualisation of the Cl, δ^{18}O, TDS and mixing proportions of the cored boreholes, obtained with the following end-members: Littorina, Glacial, Brine (deep saline) and altered meteoric (HLX28).

KLX01 (HLX28)









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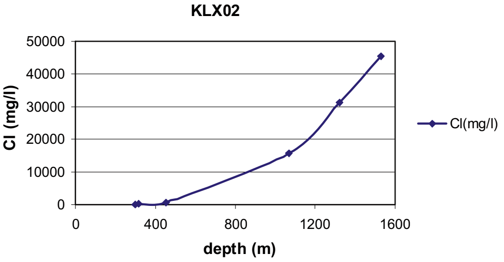

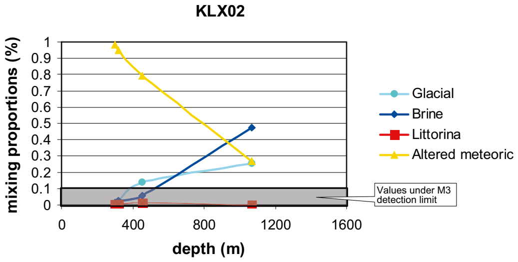

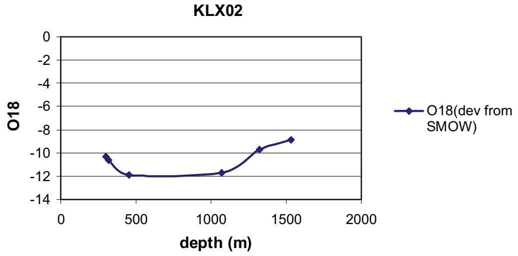

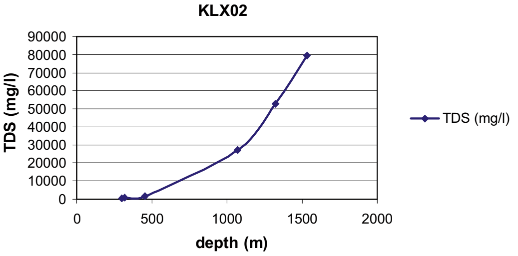

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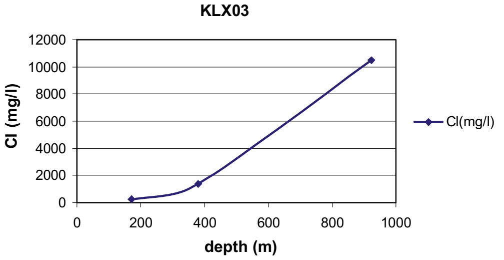

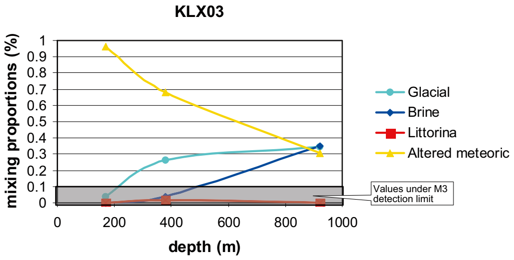

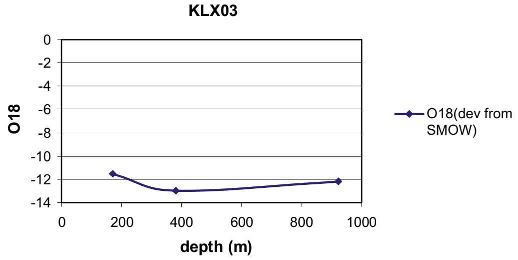

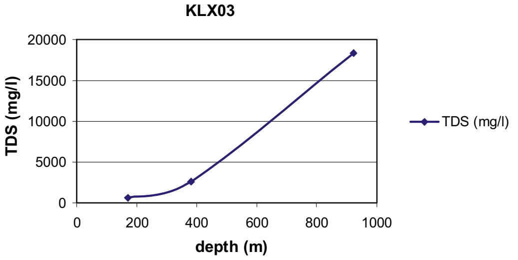

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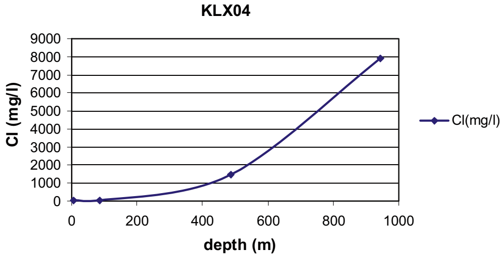

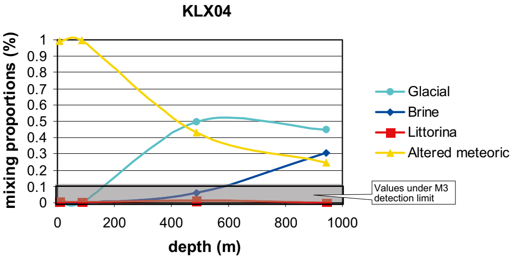

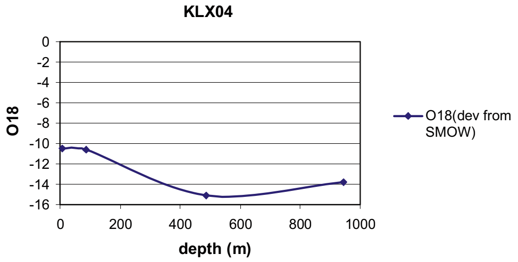

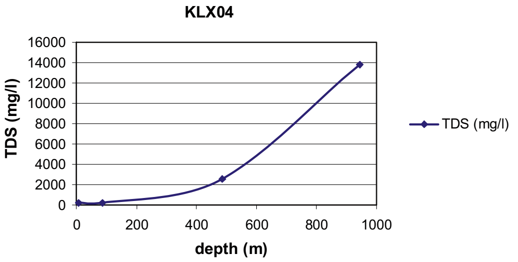

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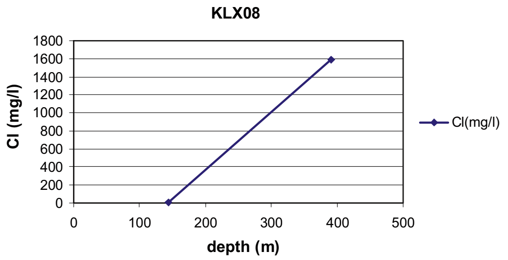

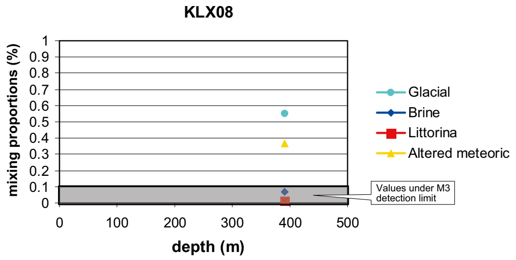

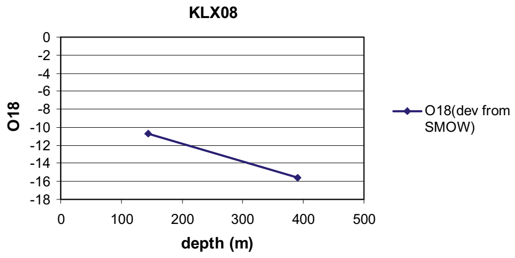

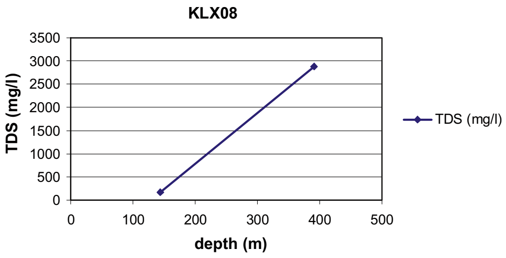

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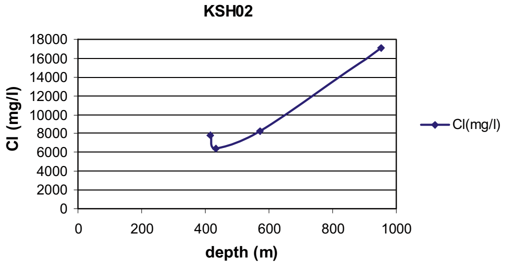

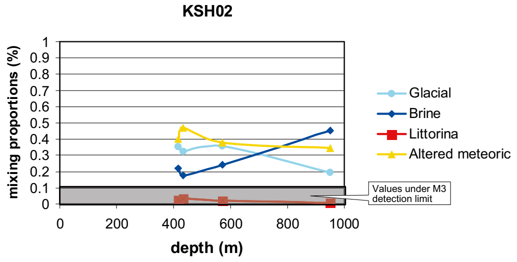

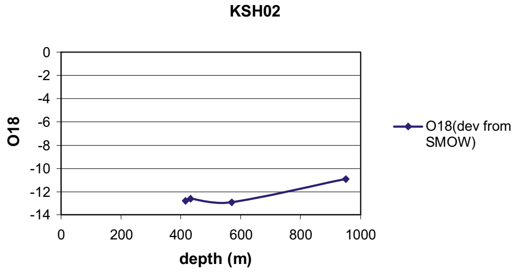

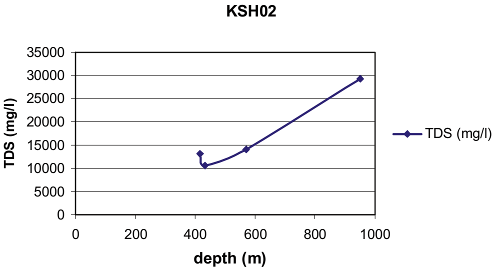

Section 2

Integrated hydrogeological and geochemical modelling of the Laxemar-Simpevarp area during the recent Holocene (last 8,000 years)

Contribution to SDM-Site Laxemar Hydrochemistry Background Report

Jorge Molinero, Joaquín Salas,
David Arcos, Lara Duro

Contents

1 Introduction and objectives

The Swedish Nuclear Fuel and Waste Management Company (SKB) is studying two alternative sites (Forsmark and Laxemar) to locate a deep geological repository for the disposal of spent fuel. One of the two sites being investigated is the Laxemar-Simpevarp area, located in the Baltic coast of Sweden about 400 km south of Stockholm. In this context, SKB is conducting a comprehensive geoscientific modelling work that is performed as a major part of the site characterisation program in Sweden. Hydrogeology and hydrochemistry constitute two of the key disciplines involved in such an effort, and coupled reactive solute transport modelling is one of the approaches selected by SKB to contribute to the overall understanding of the investigated systems. The methodology for quantitative integration of hydrogeologic and hydrochemical understanding of the Laxemar site is presented here. Large-scale and long-term palaeohydrogeochemical simulations have been performed which are able to simulate key reactive transport processes during the last 8,000 years. This work is a first attempt to assess the usefulness of reactive solute transport approach within the framework of conceptual site understanding and modelling.

The effects from the last glaciation and the consequent land uplift are the most important recent events which are likely to affect significantly the measured groundwater composition at the Laxemar-Simpevarp area. When the continental ice was melting and retreating, it is assumed that glacial melt waters were injected into the basement. After the deglaciation stage, the Littorina Sea (an ancient stage of the current Baltic Sea) that covered the area which most likely provided saline waters reaching chloride contents of about 7 g/L. Density-driven turnover is believed to be an important process during this period, and then, glacial water could have been replaced and mixed with sea water. Finally, the main part of the present Laxemar-Simpevarp area rose above the sea level about 2000 BC. Fresh water aquifers started to form and fresh water of meteoric origin mixed with previously existing groundwater /Laaksoharju et al. 1999/.

According to such a conceptual model, two distinct flow regimes must be considered in order to simulate the hydrogeochemical evolution of the Laxemar-Simpevarp area since the last glaciation: (a) Littorina sea water sinking (mainly density driven) into the bedrock with previously infiltrated glacial melt water, and (2) meteoric flushing of the system (topographically driven) to the present day conditions. The hydrogeochemical evolution of such a long-term, large scale, complex system has been numerically simulated by combining hydrogeological and reactive transport models. A comprehensive hydrogeological model has been developed to simulate the groundwater flow evolution of the Laxemar area on a regional-scale (hundreds of square kilometres) during the last 8,000 years /Hartley et al. 2007, Hunter et al. 2008/. This hydrogeological model corresponds to the model version 2.1 of the Simpevarp regional model. The model accounts for variable-density groundwater flow and incorporates the major fracture zones of the site as deterministic features. The computed flow field at several cross-sections has been extracted at different times and exported into 2D reactive transport models. Such reactive transport models incorporate key hydrogeochemical processes such as cation exchange in clay minerals, carbonates dissolution/precipitation and silicates weathering. It is worth noting that redox processes have not been included in the modelling so they are not simulated in the current version of the reactive transport calculations.

The main objectives of this work are:

(1) To evaluate quantitatively the relative importance of different reactive processes along the simulated time, as well as the impact of such hydrogeochemical process in the current groundwaters of the site.

(2) To develop and test a methodology for quantitative integration of hydrogeological and hydrochemical data and knowledge of the site.

A summary of the physico-chemical formulation of the groundwater flow and reactive transport phenomena is summarised in Chapter 2. Then, Chapter 3 shows the methodological approach and the conceptual model. Computed results are presented and discussed in Chapter 4. Finally, the main achievements and conclusions of the work are summarised in Chapter 5 of this report.

2 Formulation

2.1 Groundwater flow

Where groundwater density varies spatially, flow may be driven by difference either in fluid pressure or by unstable variations in fluid density. Assuming isothermal conditions, density-driven flows are directed from dense regions of fluid toward less dense regions.

Pressure and density-driven forces for groundwater flow can be accounted for by combining Darcy's Law and the mass balance equation, as expressed by /Voss and Provost 2003/:

$$\left(\theta\rho S_{op}+\frac{\rho}{\phi}\frac{\partial\theta}{\partial p}\right)\frac{\partial p}{\partial t}+\left(\frac{\theta}{\phi}\frac{\partial p}{\partial c}\right)\frac{\partial c}{\partial t}-\nabla\bullet\left[\left(\frac{k\rho}{\mu}\right)\bullet(\nabla p-\rho g)\right]=Q_p \qquad \text{Equation 2-1}$$

where ρ represents density; θ is the volumetric water content, S_{op}, the specific pressure storativity, ϕ, the porosity, and k, the intrinsic permeability tensor of the medium; p is pressure; g is gravitational acceleration; μ is the dynamic viscosity of the fluid; and Q_p is a fluid mass source.

Total fluid density is the sum of pure water density and solute volumetric concentration. Approximate density-models can be employed using first order Taylor expansions in C (solute mass fraction) about a base density, as suggested by /Voss and Provost 2003/:

$$\rho(C)\cong\rho_0+\frac{\partial\rho}{\partial C}\left(C-C_0\right) \qquad \text{Equation 2-2}$$

where ρ_0 is the base fluid density at base concentration, C_0 (usually, $C_0 = 0$, and the base density is that of pure water). The factor $\frac{\partial\rho}{\partial C}$ is a constant value of density change with concentration.

2.2 Reactive solute transport calculations

Coupled with groundwater flow, the movement of dissolved species is characteristic of hydrogeologic systems. Solute transport is mainly the result of the combined effects of advection, molecular diffusion and hydrodynamic dispersion. The classical mathematical treatment of such processes involves the solution of the well-known general advection-dispersion equation /Bear 1972/. In a two-dimensional domain, the equation can be written as /Samper et al. 2000, Yeh 2000/:

$$\nabla\bullet\left(\theta bD\nabla c_k\right)-bq\nabla c_k+r\left(c_k^*-c_k\right)+b\theta R=b\theta\frac{\partial c_k}{\partial t} \qquad \text{Equation 2-3}$$

where b is the transverse thickness of the two-dimensional domain; D is the dispersion tensor, which lumps the effects of molecular diffusion and hydrodynamic dispersion; c_k is the solute concentration (expressed as solute mass per unit fluid volume) of the k-th aqueous species; q is the Darcy velocity; r is the fluid source term per unit surface area; c_k^* is the solute concentration in fluid sinks/sources; and R is a chemical sink/source term.

Most hydrochemical processes in groundwater are almost instantaneous and they can be effectively considered as equilibrium reactions. The equilibrium constant relates the average number of ions pairs or complexes which are being formed. Applying the Mass-Action Law to the dissociation of the *j-th* secondary species produces Equation 2-4:

$$K_j=a_j^{-1}\prod_{i=1}^{N_c}a_i^{\nu_{ji}} \qquad \text{Equation 2-4}$$

where a_i and a_j are the thermodynamic activities of the species j and i, respectively, and ν_{ji} is the stoichiometric coefficient of *i-th* primary species in *j-th* species. This equation allows the concentration of secondary species or aqueous complexes x_j to be expressed in terms of primary species concentrations c_i according to Equation 2-5:

$$x_j=K_j^{-1}\gamma_j^{-1}\prod_{i=1}^{N_c}c_i^{\nu_{ji}}\gamma_i^{\nu_{ji}} \qquad \text{Equation 2-5}$$

where x_j and c_i are molal concentrations and γ_j and γ_i are thermodynamic activity coefficients.

Accordingly, the total dissolved concentration of a given component C_k can be written in an explicit form as a function of the concentration of the N_C dissolved primary species as in Equation 2-6 /Samper et al. 2000/:

$$C_k = c_k + \sum_{j=1}^{N_x} \nu_{jk} x_j = c_k + \sum_{j=1}^{N_x} \nu_{jk} K_j^{-1} \gamma_j^{-1} \prod_{i=1}^{N_c} c_{ji}^{\nu_{ji}} \gamma^{\nu_{ji}} \qquad \text{Equation 2-6}$$

where N_x is the number of secondary species. Notice the difference between the concentration of primary species c_k and the total dissolved concentration of the componenet C_k.

The chemical composition of an aqueous system containing N_E species can be expressed in terms of the concentrations of N_C components (primary species). This is a key point for reactive solute transport modelling by using operator splitting techniques, because instead of N_E transport equations only N_C equations have to be solved. The concentration of the N_x secondary species can be explicitly computed from the concentrations of primary species. This usually leads to a significant reduction of computing time /Lichtner et al. 1996/, but not always is more efficient than fully implicit schemes /Saaltink 1999/.

For dilute solutions (less than 1 mol/kg) the value of the activity coefficient of the *i-th* aqueous species can be calculated according to the extended Debye-Hückel approach (Equaton 2-7):

$$\log \gamma_i = -\frac{A z_1^2 (I)^{\frac{1}{2}}}{1 + B a_i (I)^{\frac{1}{2}}} + bI \qquad \text{Equation 2-7}$$

where I is the ionic strength of the solution; z_i and a_i are the electric charge and the ionic radius in solution of the *i-th* aqueous species, respectively; A and B are constants which depend on temperature and dielectric constant of water, and b is a constant determined from fitting experimental data. The values of A, B and b at different temperatures are tabulated in /Helgeson and Kirkham 1974/. The value of the ionic strength is calculated as (Equation 2-8):

$$I = \frac{1}{2} \sum_{i=1}^{N_T} c_i z_i^2 \qquad \text{Equation 2-8}$$

The activity of water can be calculated according to /Garrels and Christ 1965/ as in Equation 2-9:

$$a_{H_2O} = 1 - 0.018 \sum_{i=2}^{N_T} c_i \qquad \text{Equation 2-9}$$

where i includes all dissolved species except water.

Under equilibrium conditions, dissolution-precipitation of minerals can also be described by the Law of Mass Action as Equation 2-10

$$X_m \lambda_m K_m = \prod_{i=1}^{N_c} c_i^{\nu_{mi}^p} \gamma^{\nu_{mi}^p} \qquad \text{Equation 2-10}$$

where X_m is the molar fraction of the *m-th* solid phase, λ_m is its thermodynamic activity coefficient (X_m and λ_m are taken equal to 1 for pure phases), c_i and γ_i are the concentration and activity coeficient of the *i-th* species, υ^p_{mi} its stoichiometric coefficient in the dissolution reaction of the *m-th* solid phase, and K_m is the corresponding equilibrium constant.

However, the assumption of thermodynamic equilibrium might not hold when dealing with water-mineral interactions. This is the case, for instance, of the incongruent dissolution of primary silicates of granitic rocks (i.e. feldspars). According to /Lasaga et al. 1981/, the kinetics of mineral dissolution/precipitation processes can be evaluated by means of the expression shown in Equation 2-11:

$$r_m = \varsigma_m A_m e^{-\frac{Ea_m}{RT}} \sum_{k=1}^{N_k} K_{mk} \prod_{i=1}^{N_c+N_x} a_i^{p_{mki}} \left(\Omega_m^{\theta_{mk}} - 1\right)^{\eta_{mk}} \qquad \text{Equation 2-11}$$

where r_m is dissolution-precipitation rate (mol/m^2/ s); ς_m is equal to 1 (dissolution) or –1 (precipitation) depending on whether Ω_m is larger or smaller than 1, respectively; Ω_m is the ratio between the ion activity product and the equilibrium constant; $e^{-\frac{Ea_m}{RT}}$ is a thermodynamic factor, Ea_m is the apparent activation energy of the overall reaction process (kJ/mol); R is the gas constant (kJ/mol·T; T is absolute temperature (K); N_k is the number kinetic reactions for mineral m, (it is usually equal to 1); K_{mk} is the kinetic rate constant of *m-th* mineral in *k-th* kinetic reaction (mol/m^2/ s); A_m is the specific surface area (m^2/mol); $\prod_{i=1}^{N_c+N_x} a_i^{p_{mki}}$ accounts for the catalytic effect of some species such as H$^+$; N_c y N_x are the number of primary and secondary species, respectively; and θ_{mk} and η_{mk} are parameters of the *k-th* kinetic reaction for the *m-th* mineral, which are usually determined by experiments.

A general expression for cation exchange reaction according to the Gaines-Thomas convention is shown in Equation 2-12 /Appelo and Postma 1993/:

$$\frac{1}{\nu_i}S_i + \frac{1}{\nu_j}\left(X_{\nu_j} - S_j\right) \Leftrightarrow \frac{1}{\nu_i}\left(X_{\nu_i} - S_i\right) + \frac{1}{\nu_j}S_j \qquad \text{Equation 2-12}$$

where v_i and v_j are the stoichiometric coefficients of dissolved and interlayer cations, respectively; S_i and S_j denote dissolved cationic species and (X_{ν_i} –S_i) and (X_{ν_j} –S_j) represent exchange sites or exchange interlayer cations. Likewise, the equilibrium equation for cation exchange is obtained from the mass action law as in Equation 2-13:

$$K_{ij}^{*} = \frac{\overline{w_i}^{1/\nu_i} \bullet a_j^{1/\nu_j}}{\overline{w_j}^{1/\nu_j} \bullet a_i^{1/\nu_i}} \qquad \text{Equation 2-13}$$

where K_{ij}^{*} is the exchange coefficient, a_j is the activity of the *j-th* dissolved species and $\overline{w_i}$ is the activity of the *i-th* exchanged species.

The reactive transport problem is addressed in this model by means of a sequential iterative approach /Xu et al. 1999, Samper et al. 2000/. This technique consists in uncoupling the transport and chemical reactions. In the first step of calculation, mass transport is solved in terms of total dissolved concentrations of components accounting for respective geochemical source/sink terms. Total concentrations of components and immobile species, minerals, gases, adsorbed and exchanged species, are then calculated for every nodal point. Once transport calculations are finished, total nodal concentrations are evaluated in order to check whether they violate the chemical equilibrium (or kinetically-driven) relationships of the various geochemical processes considered in the model. If this is the case, chemical processes are solved in a node basis and concentrations are duly updated, providing the modified concentration fields which will serve as a starting point for the calculation of the next time step. The coupling between transport and chemical processes is solved by a Newton-Raphson iterative approach until reaching the prescribed (user defined) convergence criteria.

3 Methodological approach and conceptual model

3.1 Hydrogeological modelling

Within the SDM activities, complex three-dimensional hydrogeologic models have been developed in order to simulate the groundwater flow evolution of the Laxemar-Simpevarp area. The models cover a regional-scale area with a long time horizon to simulate the last 8,000 years. These hydrogeologic models account for variable-density groundwater flow and incorporate the major fracture zones of the site as deterministic features, as well as the bedrock properties derived from discrete fracture network analysis. Details of the hydrogeologic models of the Laxemar-Simpevarp area can be found in /Hartley et al. 2007, Hunter et al. 2008/. Those hydrogeologic models describe the complex palaeohydrodynamic evolution of the site and model results have been tested and calibrated by using both hydrogeologic and hydrochemical field information /Hartley et al. 2007/. To couple reactive transport processes into such a regional-scale, long-term, three-dimensional hydrogeologic model, with millions of elements, is outwith the current capabilities of available simulation tools due to the huge amount of computational resources that would be required. This is why a two-step decoupled approach has been developed which is presented in this report.

The approach is based on running the three-dimensional hydrogeologic models of the site, with a simplified geometry of the main deformation zones that want to be studied in detail by reactive transport simulations. Hydrogeologic models were solved by using CONNECTFLOW /Serco Assurance 2005/. Computed flow fields at target cross-sections were extracted at different times from the hydrogeologic models and exported into two-dimensional reactive transport models. Figure 3-1 shows the planar view with the location of 3 two-dimensional cross-sections were flow fields have been extracted from the hydrogeological model. Reactive transport simulations were solved by using the code CORE^{2D} /Samper et al. 2000/. Then, the overall transient palaeohydrogeologic evolution of the site is approximated as a series of steady-state flow fields and fully transient reactive transport simulations.

The hydrogeologic models incorporate the hydrochemical story of the site in terms of mixing fractions of 4 reference waters (Table 3-1): (1) Deep saline water that corresponds to the most saline and deep sample found at the Laxemar site (KLX02 borehole). (2) Glacial water that represents a possible melt-water composition from the last glaciation (> 11,000 BC). (3) Littorina sea water that corresponds to the theoretical composition an old stage of the Baltic sea (4000 years BC approx) with more saline waters that the current Baltic sea. (4) Altered Meteoric groundwater corresponding to a shallow groundwater sample of the Laxemar site. The chemical and geochemical parameters for these extreme waters (end-memebers) have been extracted from /Auqué et al. 2006/. These data (Table 3-1) correspond to the same values used by SKB in the safety assessment for SR-Can.

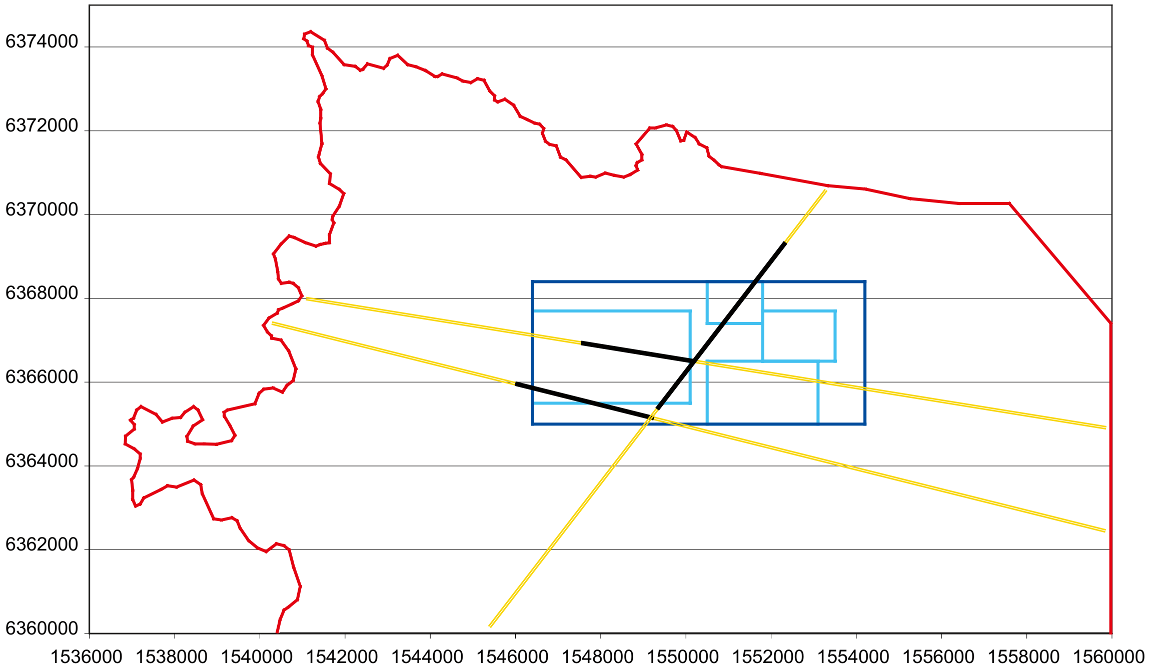

Figure 3-1. *Planar view of the top boundary of the three-dimensional hydrogeological model at the regional scale. Yellow lines show the location of the 3 cross-sections where groundwater flow fields have been extracted at different times. Red line represents the natural water divides and boundaries of the site.*

Table 3-1. Chemical composition of the reference water used to define initial and boundary conditions of the reactive transport simulations (from /Auqué et al. 2006/).

Component	Deep saline water mol/L	Littorina water mol/L	Altered Meteoric water mol/L	Glacial water mol/L
Na	3.80×10^{-1}	1.62×10^{-1}	6.70×10^{-4}	7.40×10^{-6}
K	9.00×10^{-4}	3.50×10^{-3}	7.00×10^{-5}	1.00×10^{-5}
Mg	9.00×10^{-5}	1.87×10^{-2}	1.60×10^{-4}	4.10×10^{-6}
Ca	4.94×10^{-1}	3.90×10^{-3}	9.00×10^{-4}	7.50×10^{-5}
Fe	7.00×10^{-8}	9.00×10^{-6}	1.50×10^{-5}	8.00×10^{-7}
Al	7.00×10^{-10}	1.00×10^{-7}	3.00×10^{-8}	1.90×10^{-6}
TIC	3.00×10^{-5}	1.60×10^{-3}	2.30×10^{-3}	8.90×10^{-5}
SiO_2	1.30×10^{-3}	2.00×10^{-4}	2.00×10^{-4}	2.50×10^{-4}
SO_4	9.70×10^{-3}	9.40×10^{-3}	8.00×10^{-5}	5.30×10^{-6}
Cl	$1.37\times10^{+0}$	1.86×10^{-1}	3.20×10^{-4}	1.40×10^{-5}
pH	8.00	7.94	7.37	9.25
	S.I	S.I	S.I	S.I
Calcite	0.37	0.11	–0.37	–0.87
Illite	–0.05	1.88	0.10	1.17
Chlorite	–11.02	1.79	0.06	11.88
Quartz	1.32	0.32	0.30	0.29
Albite	0.84	–0.64	–2.11	–3.55
K-feldspar	2.56	2.03	–0.07	0.92
Kaolinite	–2.73	–0.58	–0.36	–0.46

3.2 Hydrogeological and reactive transport integration

The hydrodynamic evolution of the site during the last 8,000 years has been quantitatively described by means of hydrogeological three-dimensional modelling. Then, the hydrodynamic information needed to describe the hydrogeological settings in the reactive transport modelling of the selected cross-section was delivered by the HydroNet group (N. Marsic, personnal communication). Such data delivery consisted of digital files containing the raw data of intrinsic permeabilities (m^2), kinematic porosities, Darcy velocities (m/s), pressures (Pa), salinities (kg/m^3), densities (kg/m^3), viscosities (kg/m·s) and the mixture proportions of the four end-member waters described previously (Table 3-1). The distribution of these parameters was specified in a numerical mesh of 17,480 nodes, and they are updated every 2,000 years (6000 BC, 4000 BC, 2000 BC, 0 AD and 2000 AD).

In order to integrate this information in the reactive transport models, fully heterogeneous reactive transport simulaltions (with 17,480 material zones and 17,480 initial waters) would be required. From a numerical point of view, it would be impossible in terms of computational requirements. In this way, an optimised new finite elements mesh, with 2,416 nodes and 4,500 triangular elements, has been made for the reactive transport simulations (Figures 3-2 and 3-6). As can be seen in Figure 3-2, the reactive transport numerical mesh has been refined near the surface (from 0 to 500 m depth) where the more dynamic hydrogeological system is expected and, consequently, the most aggressive geochemical conditions will occur. Then, the numerical mesh is progressively coarsened in depth. The numerical meshes have been extensively optimised down to 1,000 meters where quasi-stagnant conditons of the groundwater are expected, for the simulation time of the problem.

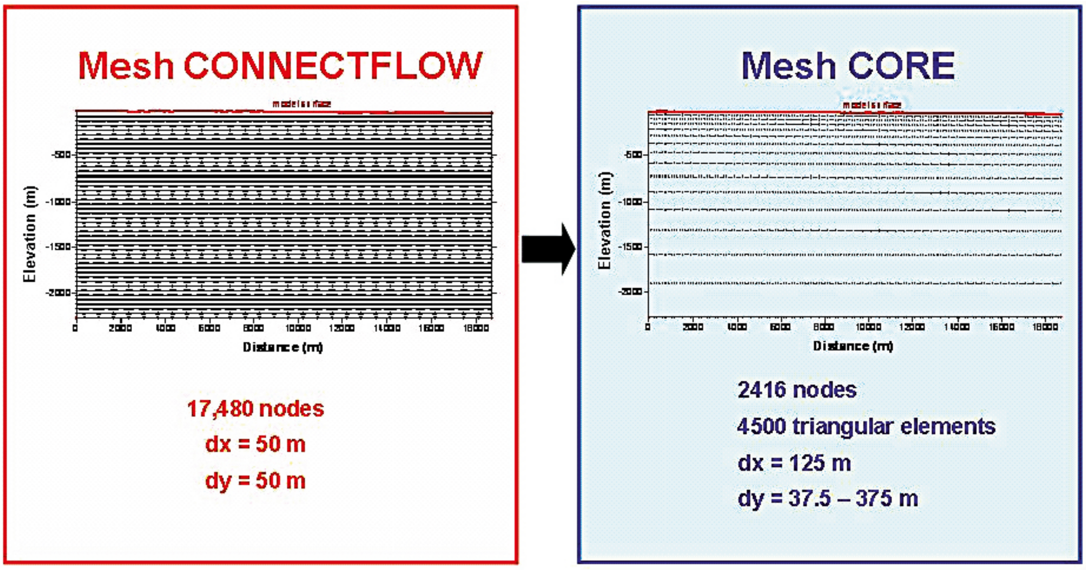

Figure 3-2. *Left: nodes of the numerical grid used for the hydrological calculations with CONNECTFLOW (as extracted from a three-dimensional model). Right: nodes of the numerical grid for the reactive transport model with CORE.*

The transfer of the hydrological information to the reactive transport models was done by using interpolation subroutines based on the method of inverse distance weighting. However, some of the hydrological parameters need to be introduced as a function of the elements (flow velocities, permeabilities, porosities, densities, dispersivities and diffusivities). Thus, new subroutines have been developed in order to assign the average value of the nodes to each element of the new (optimised) mesh, from the nodal parameters in the old (CONNECTFLOW) grid.

In order to capture the palaeohydrogeologic conditions, 5 different flow fields have been used at times: 6000 BC (to simulate the period from 6000 to 5000 BC), 4000 BC (to simulate the period from 5000 BC to 3000 AD), 2000 BC (to simulate the period from 3000 to 1000 BC), 0 AD (to simulate the period from 1000 BC to 1000 AD) and 2000 AD (to simulate the period from 1000 to 2000 AD). Flow fields are described in terms of water velocity vectors (Figure 3-3).

Hydrochemical initial and boundary conditions of the reactive transport model have been estimated based on the mixing fractions of reference waters computed by the hydrogeologic simulations, and using the chemical compositions shown in Table 3-1. Figure 3-4 shows a sketch of the methodological approach for the reactive transport simulations. The initial water composition for 6000 BC, as well as the boundary water compositions for 6000 BC (for the period since 6000 until 5000 BC), 4000 BC (for the period since 5000 until 3000 BC), 2000 BC (for the period since 3000 until 1000 BC), 0 AD (for the period since 1000 BC until 1000 AD) and 2000 AD (for the period since 1000 until 2000 AD) have been defined. The initial hydrogeochemical contions for each reactive transport modelling step are the computed results obtained in the calculations of the previous step

This methodology has been verified by comparing (1) the distribution of the hydrological parameters in both CONNECTFLOW and in CORE meshes (Figure 3-5) and (2) the hydrodynamic evolution of the 4 reference waters used as non-reacative tracers both in the CONNECTFLOW and CORE simulations. Obtained results confirm the suitability of the method.

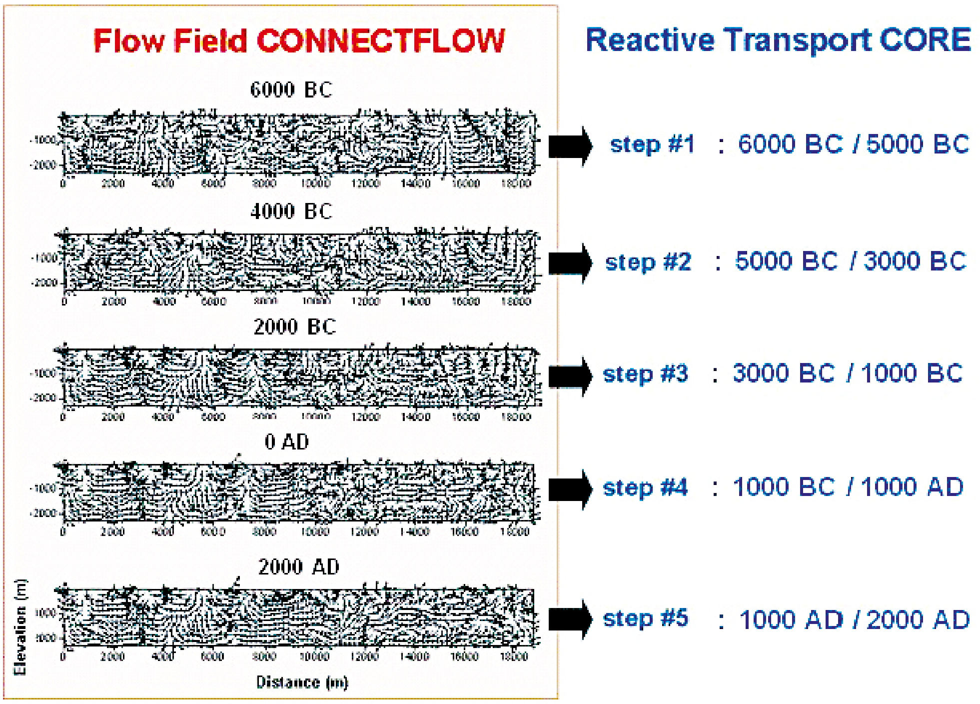

Figure 3-3. *5 steady-state flow fields used to simulate the palaeohydrogeological evolution of the last 8,000 years of the Laxemar-Simpevarp area. The flow fields have been extracted from the ConnectFlow simulations using the available regional-scale 2.1 model.*

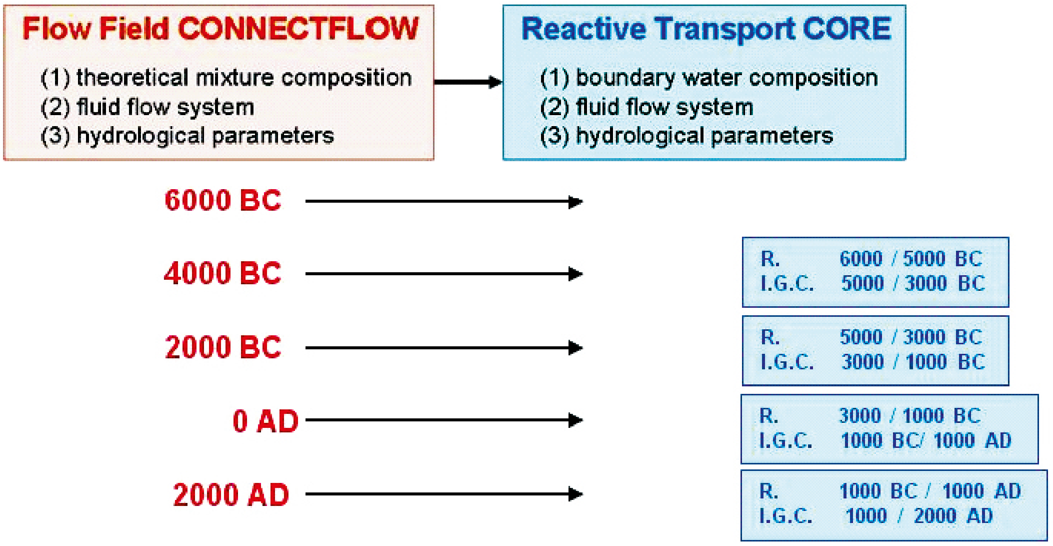

Figure 3-4. *Methodological scheme of the connection between the hydrological parameterisation obtained by the three-dimensional hydrogeological models and its implementation in the reactive transport models. R means "reactive transport simulation period". I.G.C. means "initial geochemical consitions" for the corresponding simulation period.*

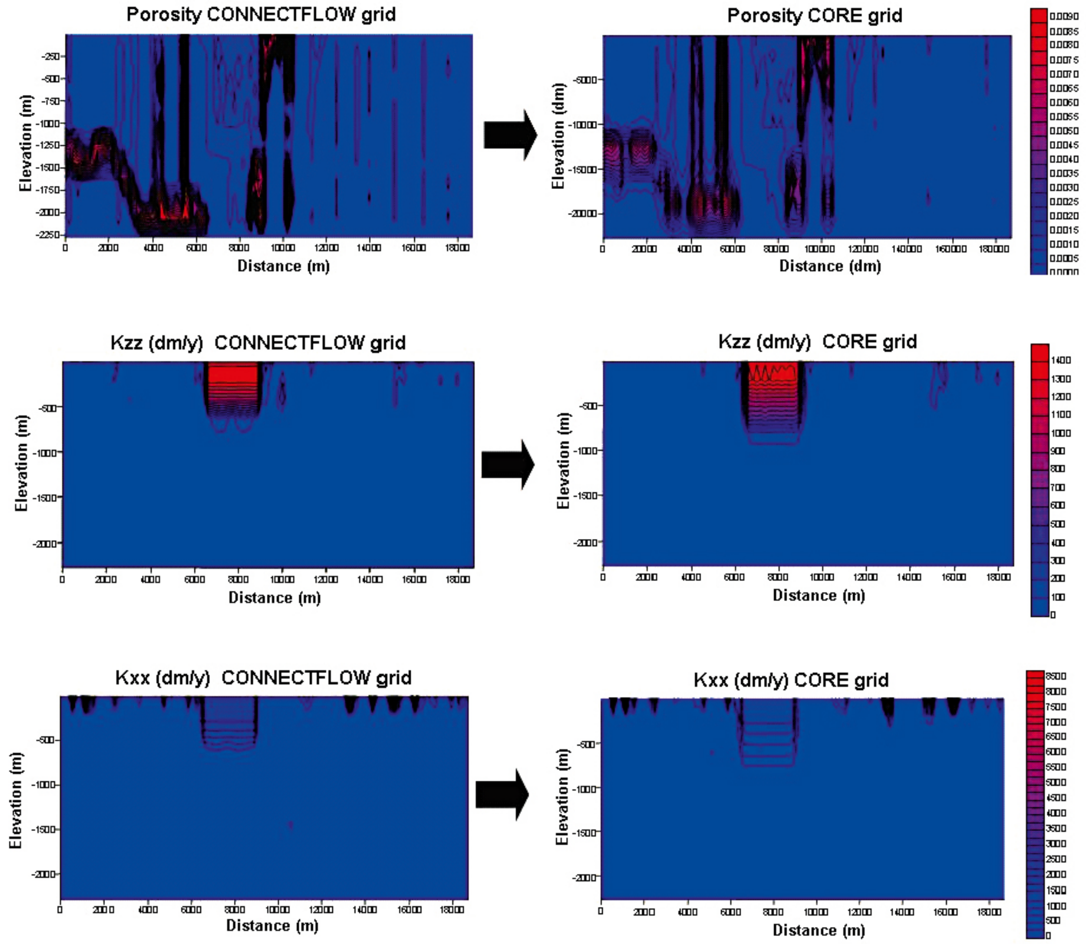

Figure 3-5. *Comparison of the spatial distribution of key parameters in the original CONNECTFLOW mesh (left) and the optimised meash for reactive transport simulations used in CORE 2D (right).*

3.3 Model domain, discretisation and hydrological parameterisation

Hydrogeochemical evolution of the last 8,000 years has been investigated by means of reactive transport simulations of a cross section which includes the deformation zone EW007A. Such a deformation zone (EW007A) is one of the major structural deterministic features in the Laxemar-Simpevarp area and runs, approximately, perpendicular to the coast of the Baltic Sea, parallel to the main topographic gradient.

The model domain is a vertical cross section, 18.700 km long and 2.275 km deep. It includes the deformation zone EW007, characterised by relatively high permeabilities. This domain has been discretised by a finite element mesh of 2,416 nodes and 4,500 triangular elements (Figure 3-6). A constant value of 125 m for Δx has been assumed whereas the Δz values are progressively increasing with respect to depth (from 37.5 m to 375.0 m). As was noted previously, this spatial discretisation has been used to optimise the computational resources required in the reactive transport simulations. Significant geochemical variations are not expected to occur at depth, in the simulatied period, where quasi-stagnant deep saline waters with relatively high densities are located.

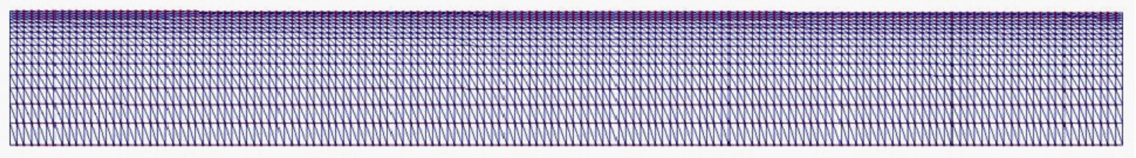

Figure 3-6. Finite elements grid used in the reactive transport simulations. It is composed of 2,416 nodes and 4,500 triangular elements.

The physico-chemical heterogeneity has been taken into account in the model by including 2,416 material zones, 2,416 initial waters and 152 boundary waters. The system has been considered as a homogeneous lithology, with a prescribed initial composition of minerals (see section 3.4).

The spatial distribution of hydrological parameters was extracted from the three-dimensional hydrogeological model (regional-scale, version 2.1). It is assumed that molecular diffusion will not play a significant role in the transport process along the simulated deformation zone, as a consequence of the relatively high advective velocities within the domain. It is worth mentioning that matrix diffusion could perhaps be relevant in the problem but it has been neglected in the current reactive transport simulaltions. The dispersivities are related to the grid spacing through the grid Peclet number /Daus et al. 1985/, knowing that the grid spacing should not exceed twice the longitudinal dispersivity in the direction of flow in ordert to avoid numerical oscillations. This is particularly important for reactive models because negative concentration values would cause the solution to fail. Another constraint is the computational cost, which can be very high in the case of reactive transport models.

3.4 Geochemical parameterisation and processes

In order to ascertain the main geochemical mechanisms which control the evolution of water composition, two kinds of simulations were performed: (a) non-reactive and (b) reactive transport simulations. The reactive transport models take into account homogeneous aqueous processes, calcite and silicates dissolution/precipitation reactions and cation exchange processes (Table 3-2 shows a summary of the hydrogeochemical processes included in the reactive transport simulations).

The geochemical system has been described by means of twelve primary species, eleven additional aqueous complexes and seven minerals (Table 3-2). All aqueous processes and cation exchange reactions are treated assuming the local equilibrium approach. The equilibrium constants for the aqueous speciation and mineral solubility were those from the EQ3NR thermodynamic database /Wolery 1992/.

The initial water compositions have been defined in each node as a non-reactive mixture of the 4 reference waters: (a) Deep saline, (b) Littorina, (c) Altered meteoric and (d) Glacial (Table 3-1). The initial proportions of the mixture have been prescribed consistently with the three-dimensional hydrogeological model of Laxemar (regional-scale, version 2.1). The speciation of these waters, and the subsequent selection of the primary species and the aqueous complexes, has been performed using the PHREEQC code /Parkhurst 1995/.

The reactive mineral phases have been selected according to the mineral composition of the open fracture fillings reported in the site /Drake and Tullborg 2007/. Calcite, chlorite, quartz, plagioclase and K-feldspar have been considered as the reactive minerals in the calculations, representing the controlling mineral phases at the start of the simulations (6000 BC). In addition, illite and kaolinite have been included as mineral phases that could precipitate during the simulation time, as a result of the rock weathering.

Table 3-2. Primary aqueous species, aqueous complexes, minerals, kinetic rate constants and cation exchange reactions used in the geochemical conceptual model. The mineral equilibrium constants were taken from the EQ3NR database (version R10, /Wolery 1992/), and the selectivity coefficients of the cation exchange reactions have been calculated from analytical data of the Swedish sites.

Primary species:

H_2O, H^+, HCO_3^-, $Al(OH)_4^-$, $SiO_2(aq)$, Fe^{2+}, Na^+, Ca^{2+}, K^+, Mg^{2+}, SO_4^{2-}, Cl^-

Aqueous complexes:

OH^-, $CO_2(aq)$, CO_3^{2-}, $FeCl^+$, Al^{3+}, $Al(OH)_3(aq)$, $H_3SiO_4^-$, $CaCO_3(aq)$, $CaHCO_3^+$, $CaSO_4(aq)$, $NaHCO_3(aq)$

Mineral reactions:

Calcite	$CaCO_3(s) + H^+ \leftrightarrow Ca^{2+} + HCO_3^-$	($\log K_{25} = -1.85$)
Quartz	$SiO_2(s) \leftrightarrow SiO_2(aq)$	($\log K_{25} = -3.99$)
Kaolinite	$Al_2Si_2O_5(OH)_4(s) + 6\ H^+ \leftrightarrow 2\ Al^{3+} + 2\ SiO_2(aq) + 5\ H_2O$	($\log K_{25} = +5.10$)
Chlorite	$Fe_{1.67}Mg_{3.33}Al_2Si_3O_{10}(OH)_8(s) + 16H^+ \leftrightarrow 2Al^{3+} + 3SiO_2(aq) + 1.67Fe^{2+} + 3.33Mg^{2+} + 12H_2O$	($\log K_{25} = +53.9$)
Plagioclase	$Ca_{0.55}Na_{0.45}Al_{1.5}Si_{2.5}O_8(s) + 6H^+ \leftrightarrow 1.5Al^{3+} + 2.5SiO_2(aq) + 0.5Na^+ + 0.55Ca^{2+} + 3H_2O$	($\log K_{25} = +14.1$)
Illite	$K_{0.6}Mg_{0.25}Al_{1.8}Al_{0.5}Si_{3.5}O_{10}(OH)_2(s) + 8H^+ \leftrightarrow 2.3Al^{3+} + 3.5SiO_2(aq) + 0.6K^+ + 0.25Mg^{2+} + 5H_2O$	($\log K_{25} = +7.06$)
K-feldspar	$KAlSi_3O_8(s) + 4\ H^+ \leftrightarrow Al^{3+} + 3\ SiO_2(aq) + K^+ + 2\ H_2O$	($\log K_{25} = -1.13$)

Kinetic rate constants (25°C) and reference:

Plagioclase	$(7.5 \cdot 10^{-10} \cdot a_H{}^{0.5}) + (1.2 \cdot 10^{-14} \cdot a_H{}^{-0.30})$	/Chou and Wollast 1985, Casey et al. 1991/
Kaolinite	$(1.7 \cdot 10^{-11} \cdot a_H{}^{0.5}) + (2.5 \cdot 10^{-17} \cdot a_H{}^{-0.3})$	/Wieland and Stumm 1992, Ganor et al. 1995/
K-feldspar	$(10^{-10} \cdot a_H{}^{0.5}) + (2.5 \cdot 10^{-17} \cdot a_H{}^{-0.45})$	/Schweda 1989, Blum and Stillings 1995/

Reactive surface áreas:

Plagioclase	10^{-5} dm² mineral / dm³ of porous médium
Kaolinite	10^{-2} dm² mineral / dm³ of porous médium
K-feldspar	10^{-2} dm² mineral / dm³ of porous médium

Cation exchange reactions:

$Na^+ + ½\ CaX_2 = ½\ Ca^{2+} + NaX$	($\log K_{Me/Ca} = -1.706$)
$Mg^{2+} + CaX_2 = Ca^{2+} + MgX_2$	($\log K_{Me/Ca} = -0.007$)
$K^+ + ½\ CaX_2 = ½\ Ca^{2+} + KX$	($\log K_{Me/Ca} = -0.036$)

Calcite and quartz dissolution/precipitation have been modelled under local equilibrium approach, due to its relatively fast reaction velocity and according to the saturation state of the end-member waters (Table 3-1). On the other hand, plagioclase, K-Feldspar and kaolinite dissolution/precipitation have been treated under a kinetic approach (Table 3-2).

There is no available information about the reactive surface areas of the different minerals, so they have been estimated. The values of specific surfaces used in the simulations are listed in Table 3-2. In the case of plagioclase, a low value of the reactive surface area (e.g. 10^{-5} dm²/dm³ of rock) has been selected in order to minimise the contribution of plagioclase dissolution in the model. Plagioclase is not a common mineral in the open fracture fillings, even if it is a major component of the rock matrix.

Cation exchange processes have also been included in the simulations. The cations considered in the exchange reactions have been Na^+, Ca^{2+}, Mg^{2+} and K^+ (Table 3-1). The cation exchange capacity and the exchanger composition have been measured in a few boreholes of the site. The distribution for the CEC values has been initially tested considering analytical data from solid samples of the Laxemar area (KLX 02, KLX 03, KLX 04 and KLX 05 boreholes, at depths of 200–700 m, and with a grain size smaller than 0.1 mm and 1.5 mm; Table 3-3). The selectivity coefficients used in this model correspond to the values derived from field data of the Forsmark site /Molinero et al. 2008/ because no data from Laxemar was available at the time of making the current modelling work.

Table 3-3. Exchange capacity of the cation (meq/100 g soil) depending on the grain size of the solid sample (analytical samples from Laxemar; 200 m depth).

Cation exchange capacity (meq/100 g soil)		
Species	**0.1 mm**	**1.5 mm**
NaX	1.5	0.4
KX	4.3	1.3
CaX_2	42.4	16.6 / 2.0
MgX_2	5.0	1.6
CEC	53.2	19.9 / 5.3

3.5 Initial and boundary conditions

The assignment of initial and the boundary waters in the model has been already described in section 3.2.

Flow rates computed with the three-dimensional hydrogeological model (regional-scale, version 2.1) have been described on the top, bottom and the two lateral boundaries of the reactive transport model. The boundary conditions are duly updated in each palaeohydrogeological period (Figure 3-4).

Solute flux associated with the corresponding water flux has been considered as the boundary conditions related to the solute transport equations. A prescribed concentration boundary condition was tested (for the upper boundary) in previous setting-up runs of the model, but unrealistic results and numerical problems were obtained. This is why such a boundary conditions option was not further used in the reactive transport simulations. The main reason to get such unrealistic results with a prescribed concentration boundary condition is the relatively large size of elements in this large-scale simulation. A prescribed concentration boundary condition on the top produced "unrealistic" larger penetrations of both Littorina and meteoric waters.

3.6 Simulated time periods

The reactive transport simulations cover 8000 years, since 6000 BC up to the present day (2000 AD). In order to integrate the hydrological data obtained from the three-dimensional hydrogeologic models, calculations have been performed in sequential steps, updating the parametrisation each 2,000 years, except in the initial and final steps of 1,000 years.

$CORE^{2D}$ code computes authomatically the time step of the simualtions according to optimisation algorithms. Minimum (initial) time step were prescribed to 0.1 days. Maximum allowed time step in the simulations was 1 year. However, when it is numerically required, the code automatically re-calculates lower time steps, in order to improve numerical convergence.

4 Results of the reactive transport model

4.1 Conservative transport model simulation

The hydrodynamic evolution of the 4 reference waters (Deep saline, Littorina, Glacial and Altered meteoric) has been analysed by means of solving solute transport equations of four non-reactive tracers (Figure 4-1).

Initially (6000 BC), deep saline water is present below the –1,000 m of elevation, and it is assumed that glacial melt-waters occupy most of the upper half of the bedrock domain (Figure 4-1).

During the period from 6000 until 5000 BC, density-driven infiltration of the Littorina seawaters advances in the eastern side and mainly penetrates the EW007 deformation zone.

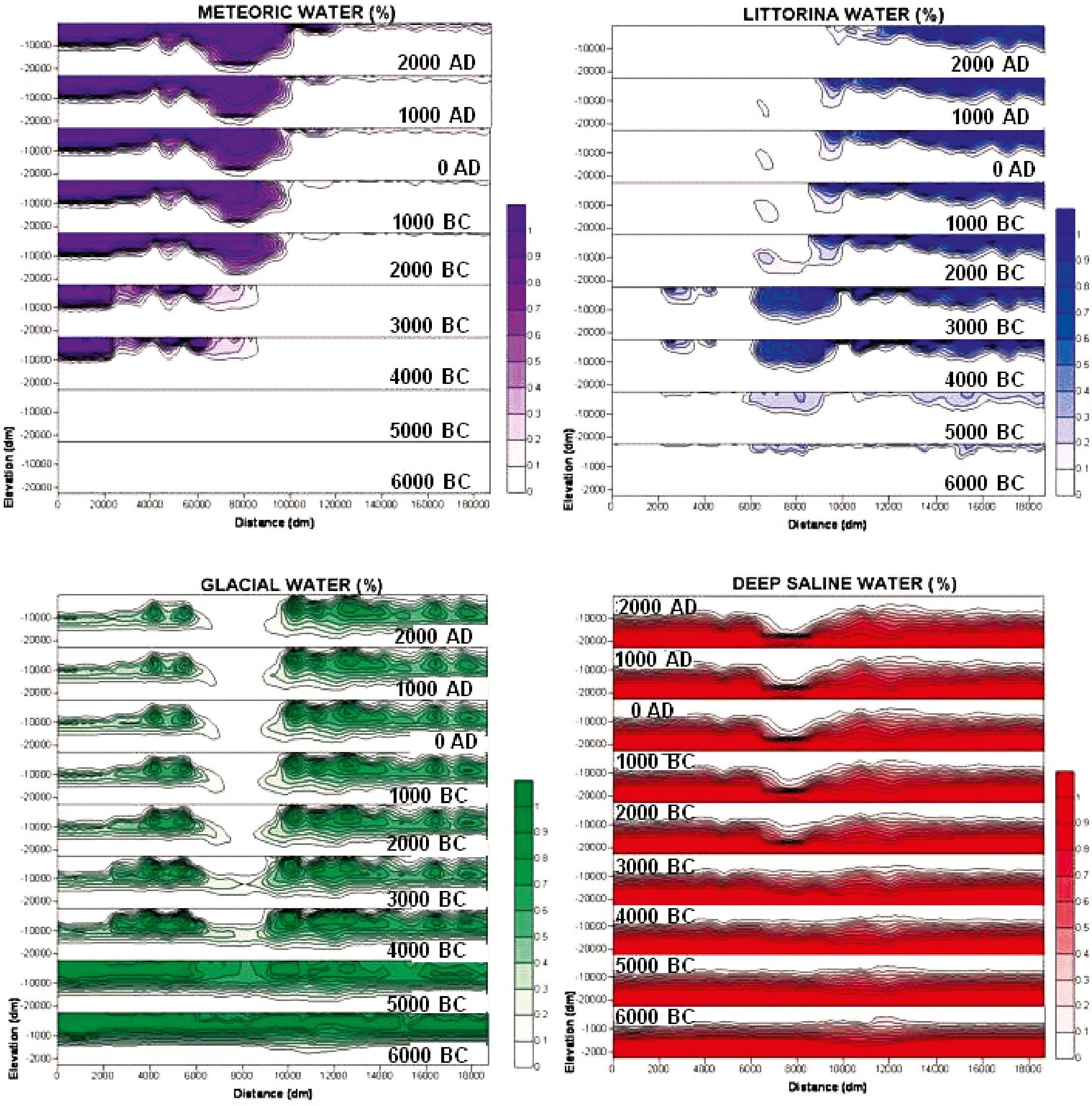

Figure 4-1. Computed distribution of the 4 reference waters. Results show the palaeohydrogeological evolution of the system from 6000 BC to AD to 2000 AD.

However, it is diluted by fresh groundwater of glacial origin, initially present in the bedrock. Consequently, the proportion of the Littorina seawater in the mixture does not exceed 30%.

The infiltration of meteoric water began during the period from 5000 until 4000 BC (Figure 4-1). It is focused on the continental side of the domain (left). As a consequence, the old glacial water located in this area is washed-out. During this time, the infiltration of Littorina water continues on the EW007 deformation zone and on the eastern zone of the model (Figure 4-1). These processes continue until 3000 BC.

During the period from 3000 until 2000 BC, the coast line moves back to the East (right in Figure 4-1), and the EW007 deformation zone is exposed to sub-aerial conditions. In this way, meteoric waters preferentially infiltrate this area, coinciding with the most permeable zones. As a consequence, the local Littorina and glacial waters are diluted and eventually washed out of the system.

Finally, during the period from 2000 BC until 2000 AD, the composition of the mixed groundwaters remains relatively stable, reaching a pseudo steady-state. The infiltration of meteoric water is being progressively extended in the model domain. However, seawater remains as the main contributior of the groundwater composition in the eastern zone of the model, corresponding to the current Baltic coastal area. Deep saline waters remain relatively stable during all the modelling time, as a consequence of their high densities.

4.2 Reactive transport modelling: evaluation of the role of geochemical processes

According to the current conceptual model for the site, it is thought that mineral dissolution/precipitation and cation exchange reactions are the main geochemical processes influencing the evolution of the concentrations of the major dissolved species and the pH of the system (see /Laaksoharju et al. 2009/). Figures 4-2 to 4-7 show computed mineral dissolution/precipitation in the modelled domain. It is woth mentioning that the current model do not account for redox processes, so pyrite dissolution is not included in the model.

Silicate weathering processes in the granitic bedrock are reproduced in the numerical models. It can be seen in Figures 4-2 to 4-6 that plagioclase and chlorite dissolution is computed at the same time that quartz and clay minerals (illite) precipitate in the shallowest areas, where the meteoric waters are directly interacting with the granitic rock.

Plagioclase dissolution is preferentially focused where the glacial waters are the main component of the groundwaters (Figure. 4-2). These solutions are characterised by relatively high pH values (> 9.0) and the lowest calcium concentrations. In these circumstances, calcite and plagioclase are undersaturated in these waters (both are the only modelled mineral phases whose dissolution can supply calcium to the aqueous solution; Table 3-1). Due to the relatively high pH values of these waters, the amount of calcium supplied by calcite dissolution is not very significant. Consequently, the aqueous solution remains undersaturated with respect to plagioclase, which is preferentially dissolved.

Chlorite dissolution/precipitation preferentially occurs close to the surface, due to the recharge of the meteoric water. As a consequence of the higher aluminium concentrations (Table 3-1), the glacial waters are heavily oversaturated with respect to chlorite. In this way, during the previous period of the modelling time (before the years 6000 BC), chlorite precipitated as a major component of the open fracture fillings. On the other hand, the meteoric waters are practically in equilibrium with respect to chlorite (in contrast with the Littorina waters, slightly oversaturated, and the deep saline waters, strongly undersaturated). As a result of the mixing processes, chlorite dissolves according to the evolution of the meteoric water front (Figure 4-3).

Illite and quartz precipitation preferentially occurs in the shallow zones of the model domain. During the period since 6000 until 5000 BC, the precipitation is a consequence of the infiltration of glacial waters, which are slightly oversaturated with respect to both minerals (Table 3-1; Figures 4-4 and 4-5), in the western zone of the domain. Later, the precipitation is a consequence of (a) the infiltration of the Littorina seawaters in the EW007 deformation zone (6000 until 2000 BC) and, locally, in the eastern zone and, (b) the infiltration of the meteoric waters in the western zone of the domain and in the EW007 deformation zone (2000 BC until 2000 AD). Meteoric waters are almost in equilibrium with respect to illite and quartz. However, their saturation states increase as a consequence of chlorite dissolution, and the consequent increase of the Si and Al concentrations and the pH values (Figures 4-4 and 4-5).

During the period from 6000 until 2000 BC, calcite precipitation occurs in the shallow zone of the EW007 deformation zone and, locally, in the eastern zone of the domain, as a consequence of the density-driven infiltration of the Littorina seawaters (Figure 4-6). In general, calcite dissolution is also focused in the shallowest zones (between 0 m and –250 m), in the central and in the western zones of the domain, where the infiltration of the meteoric and the glacial waters is effective (both are undersaturated with respect to this mineral; Table 3-1). The dissolution releases aqueous calcium and alkalinity to the groundwater, which washes-out and mixes with the groundwater previously located in the model domain (Littorina and deep saline water -which are oversaturated with respect to calcite and glacial waters). As a result, calcite precipitates down to –250 m, decreasing the pH of the solution about one unit. In these circumstances, kaolinite saturation increases (it was initially undersaturated in the 4 reference waters; Table 3-1), precipitating accordingly to the calcite precipitation.

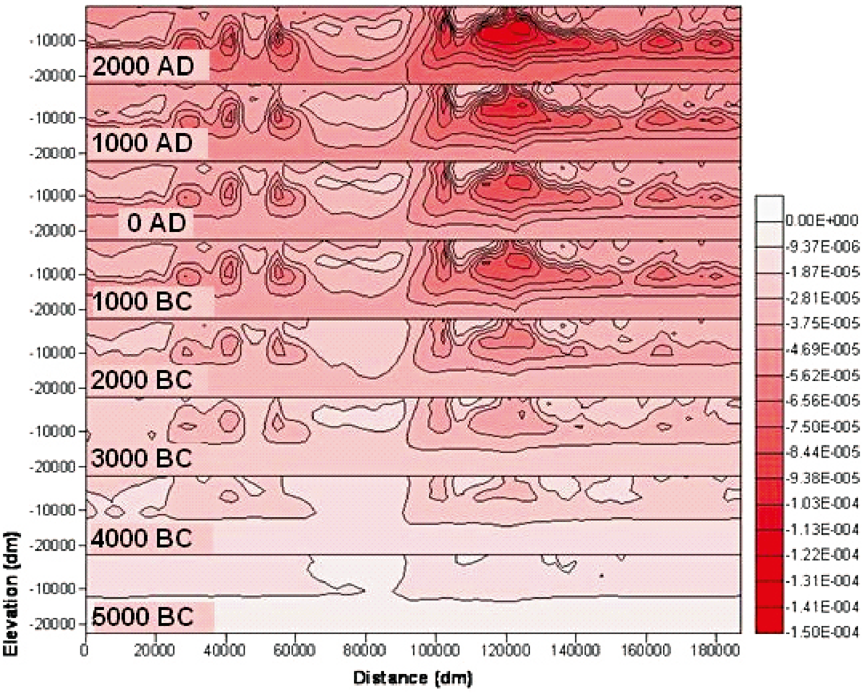

Figure 4-2. *Cumulative mass of dissolved plagioclase (mol/L of solution) obtained with the reactive transport model.*

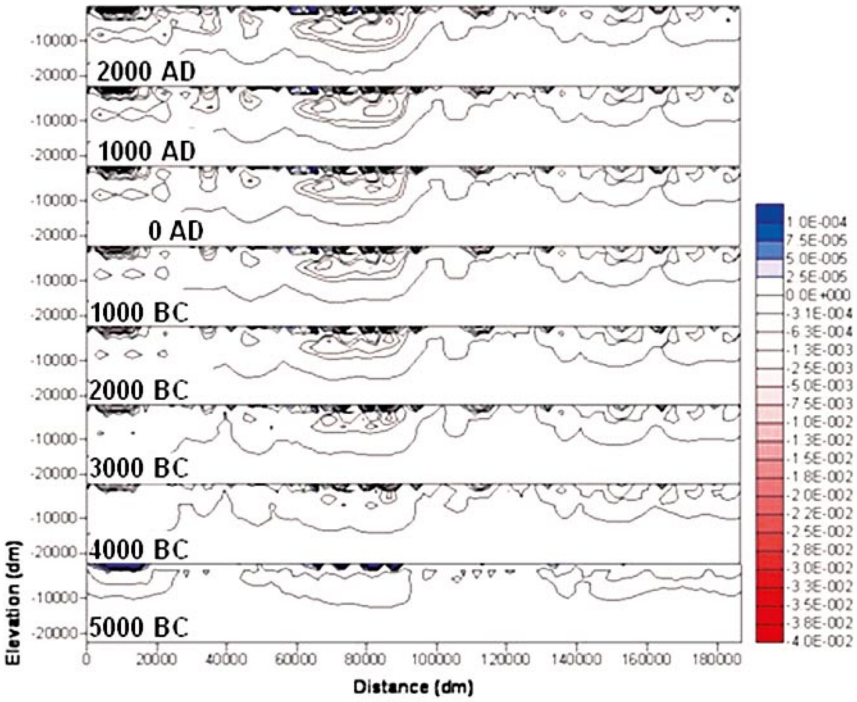

Figure 4-3. *Cumulative mass of dissolved (–; colour red) or precipitated (+; colour blue) chlorite (mol/L) obtained with the reactive transport model.*

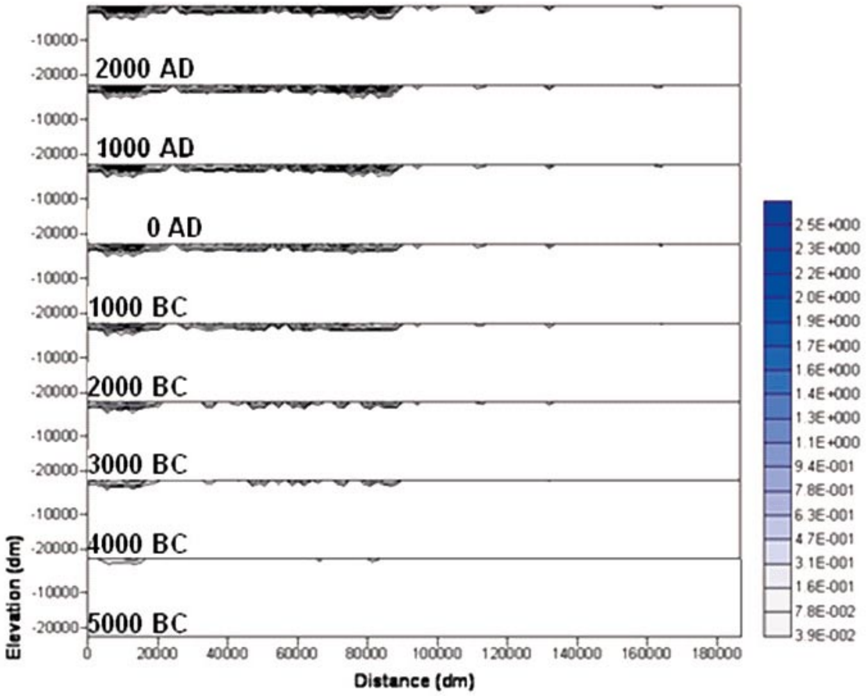

Figure 4-4. *Cumulative mass of precipitated quartz (mol/L) obtained with the reactive transport model.*

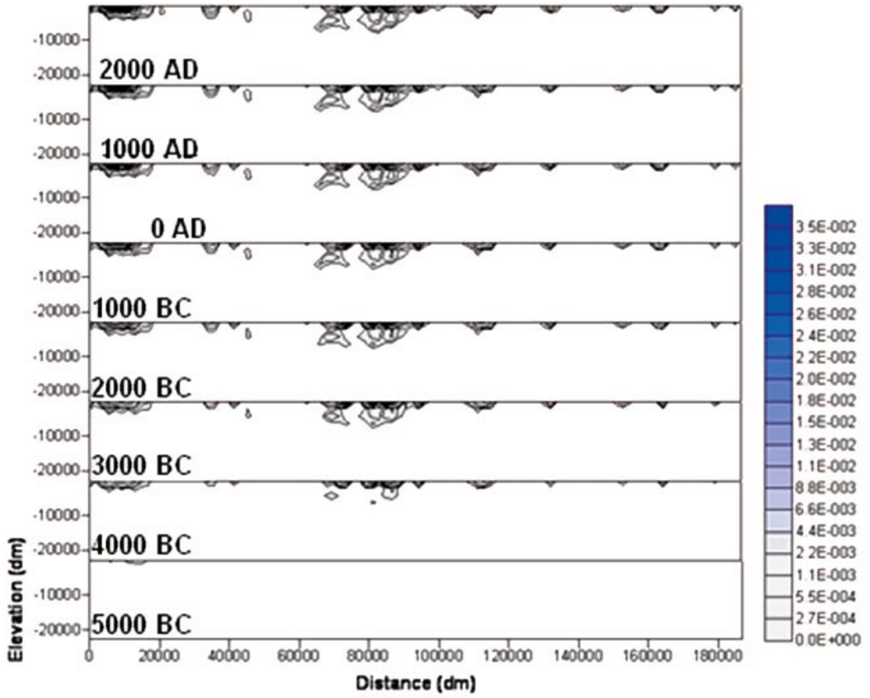

Figure 4-5. *Cumulative mass of precipitated illite (mol/L) obtained with the reactive transport model.*

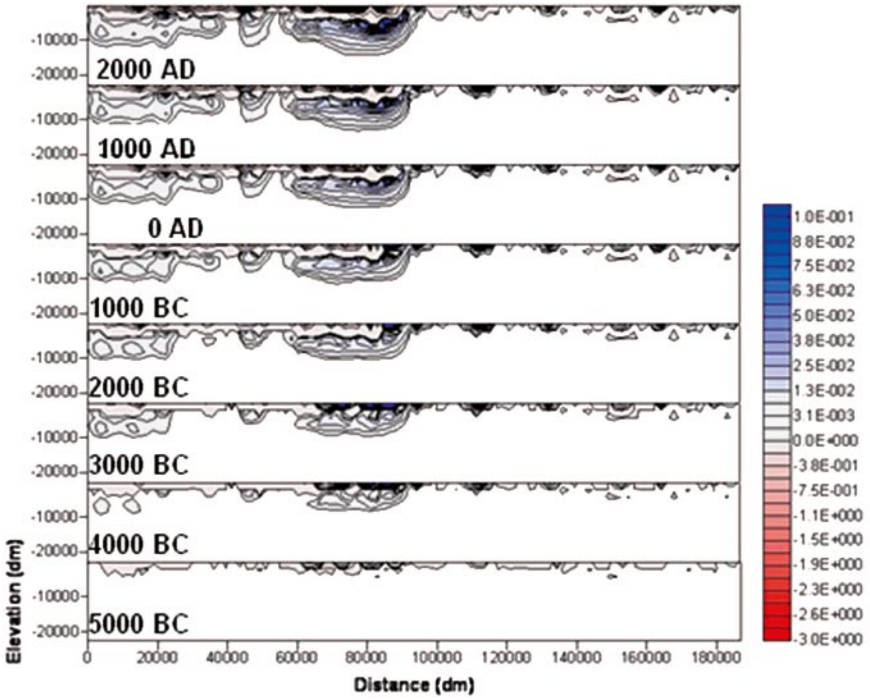

Figure 4-6. *Cumulative mass of dissolved (–; colour red) or precipitated (+; colour blue) calcite (mol/L) obtained with the reactive transport model.*

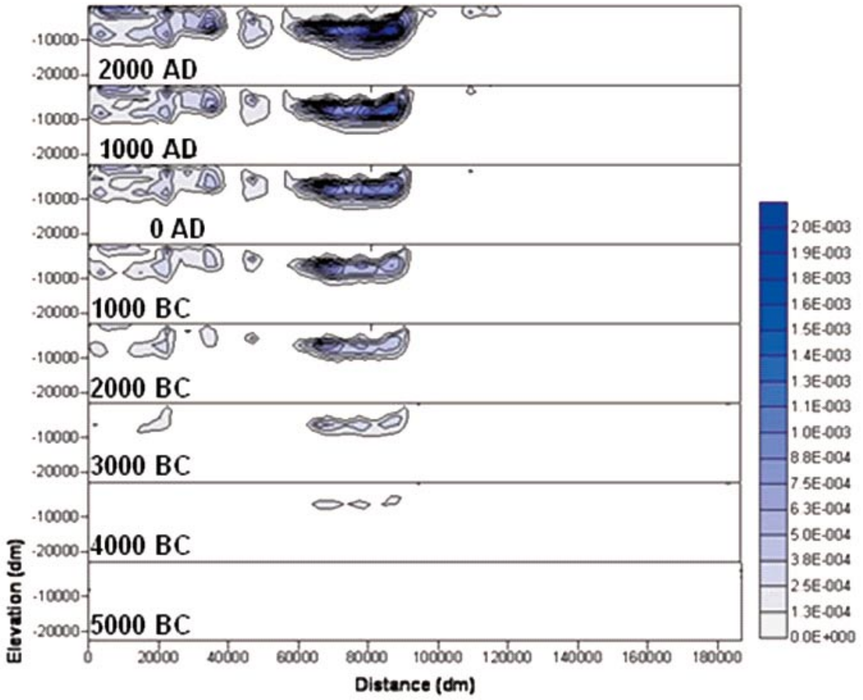

Figure 4-7. *Cumulative mass of precipitated kaolinite (mol/L) obtained with the reactive transport model.*

Additional to the fluid flow and the mixing processes, calcite dissolution/precipitation and silicate weathering reactions modify the geochemical nature of groundwaters. Comparing the distribution of the computed "conservative" pH (as a result of pure mixing processes and the fluid flow) and of the reactive pH (with chemical reactions it can be seen that the pH values increase in the shallowest areas of the EW007 deformation zone and the western areas of the domain, as a consequence of calcite and chlorite dissolution and quartz and illite precipitation (Figure 4-8). A slightly increase of the pH values in the eastern zone of the model can be observed, where plagioclase is preferentially dissolved. In accordance with calcite and kaolinite precipitation, an important decrease of the pH is also observed.

In the eastern zone of the domain (right side in the figures), above –1,000 m, the pH values obtained by the reactive transport model are lower than those obtained by the conservative transport model (Figure 4-8). This result is not associated with the mineral reactions included in the calculations, and is spatially situated in the most important zone of infiltration of the Littorina seawater. In fact, this process is associated with the cation exchange reactions, which are described later.

In the eastern zone of the domain (coinciding with the most important area of the infiltration of the Littorina waters), cation exchange reactions are the dominating geochemical mechanisms. In general, an excess of magnesium (with respect to the expected conservative values) has been calculated in groundwaters (Figure 4-9). Those are linked with a deficit of calcium, potassium and sodium. During the event of the Littorina water infiltration (6000 until 2000 BC), magnesium was fixed in the solid exchanger. Later on, as a consequence of the palaeogeographical evolution of this area, the infiltration of the meteoric waters occurs in the superficial zone. In this way, the magnesium previously fixed was exchanged by others cationic species, increasing its concentration in groundwaters.

In the area of the EW007 deformation zone (where meteoric waters have been preferentially infiltrated since 4000 BC), an excess of magnesium, sodium and potassium has been obtained, in contrast of a deficit of calcium (Figure 4-9). In this area, the volumetric rate of meteoric water infiltration is larger than in other parts of the domain. In this way, the evolution in the composition of the solid exchanger has allowed calcium fixation and release of sodium, potassium and magnesium to groundwater.

Between –1,000 m and –2,000 m elevation, an excess of calcium and sodium in groundwaters has been calculated by the reactive transport model (with respect to the results obtained by the non-reactive transport model; Figure 4-9). This zone corresponds to the fluctuation area of the front between (1) the deep saline waters and (2) the meteoric waters or the Littorina seawaters. As a consequence of the wash-out of the deep saline waters, which are being displaced by the meteoric or the Littorina waters, the cation exchange reactions releases calcium and sodium from the solid exchanger increasing their concentrations in the groundwater.

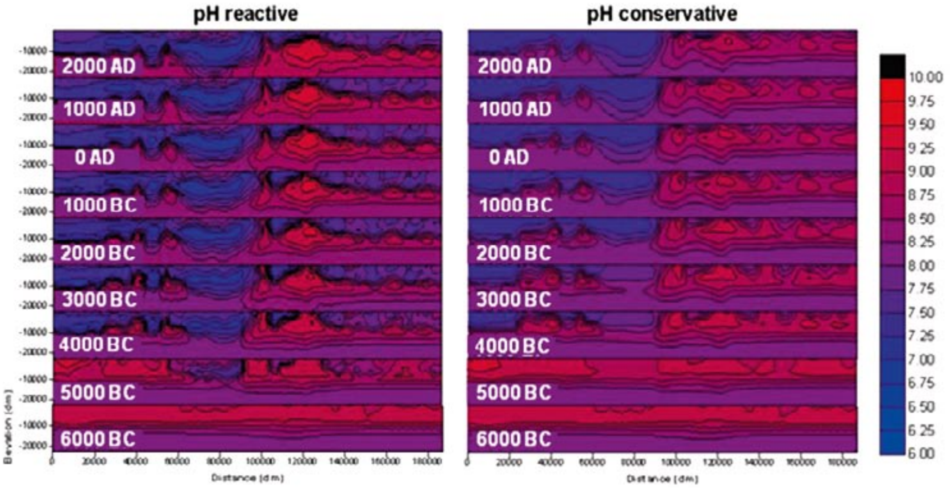

Figure 4-8. *Computed distribution of the pH values obtained by the reactive transport model and by the conservative transport model.*

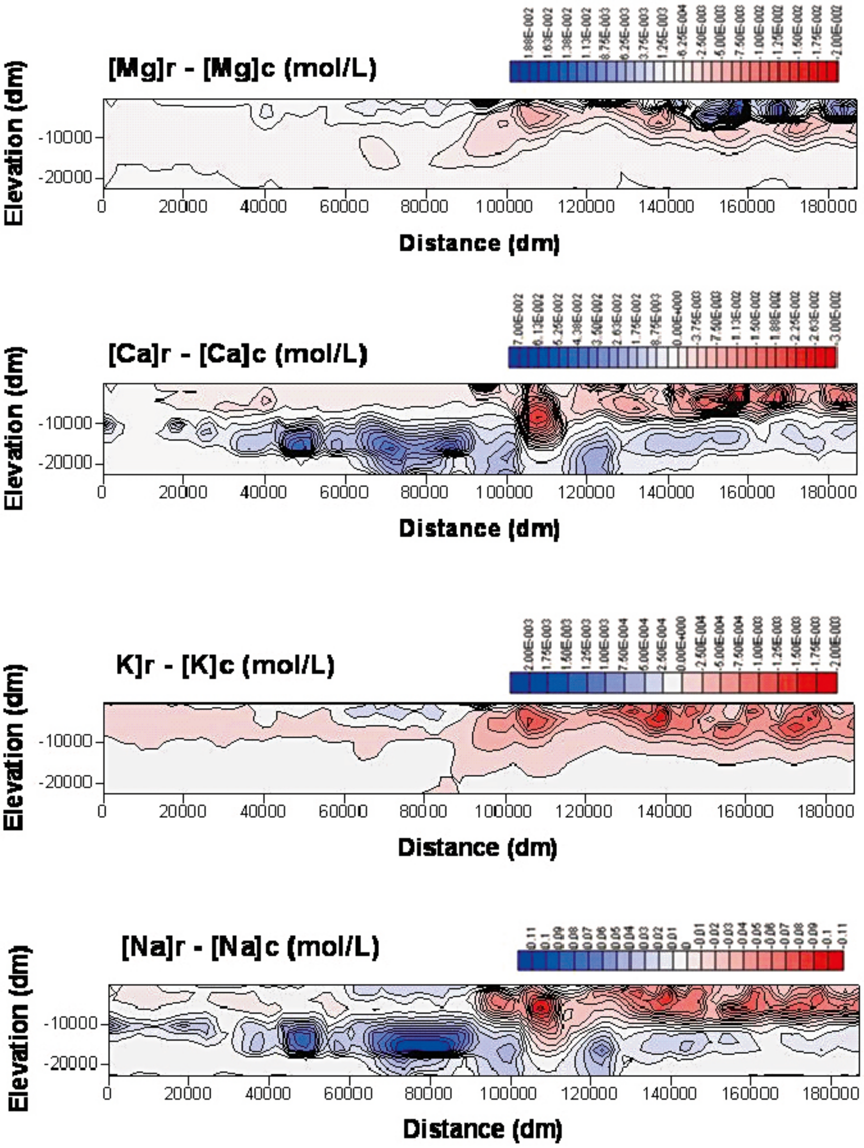

Figure 4-9. *Computed distribution of the differences between the reactive (subindex r) and the non-reactive (subindex c) concentrations obtained for magnesium, calcium, and potassium and sodium aqueous species (2000 AD).*

4.3 Reactive transport modelling: geochemical evolution in the EW007 deformation zone

In order to analyse the geochemical evolution within the EW007 deformation zone, computed results have been analysed in a vertical section located in the center of such a deformation zone within the numerical model.

Looking at the computed palaeohydrogeological evolution of the zone, 8,000 years ago (6000 BC), the shallow groundwater was a mixture between glacial waters (80–70%) and Littorina seawater (20–30%). The proportion of glacial water increases with depth up to –1,000 m, where the contribution of the deep saline waters begins to be significant. Such an initial groundwater distribution controls the evolution of the solute concentrations within the deformation zone (Figure 4-10). During the period since 5000 until 3000 BC, the infiltration of Littorina seawater was effective in this zone. Consequently, aqueous species concentrations increase in the groundwaters (above –700 m). Later, and up to the present day, meteoric waters infiltrate from the surface. Consequently, the concentrations of cation species are progressively decreasing (Figure 4-10).

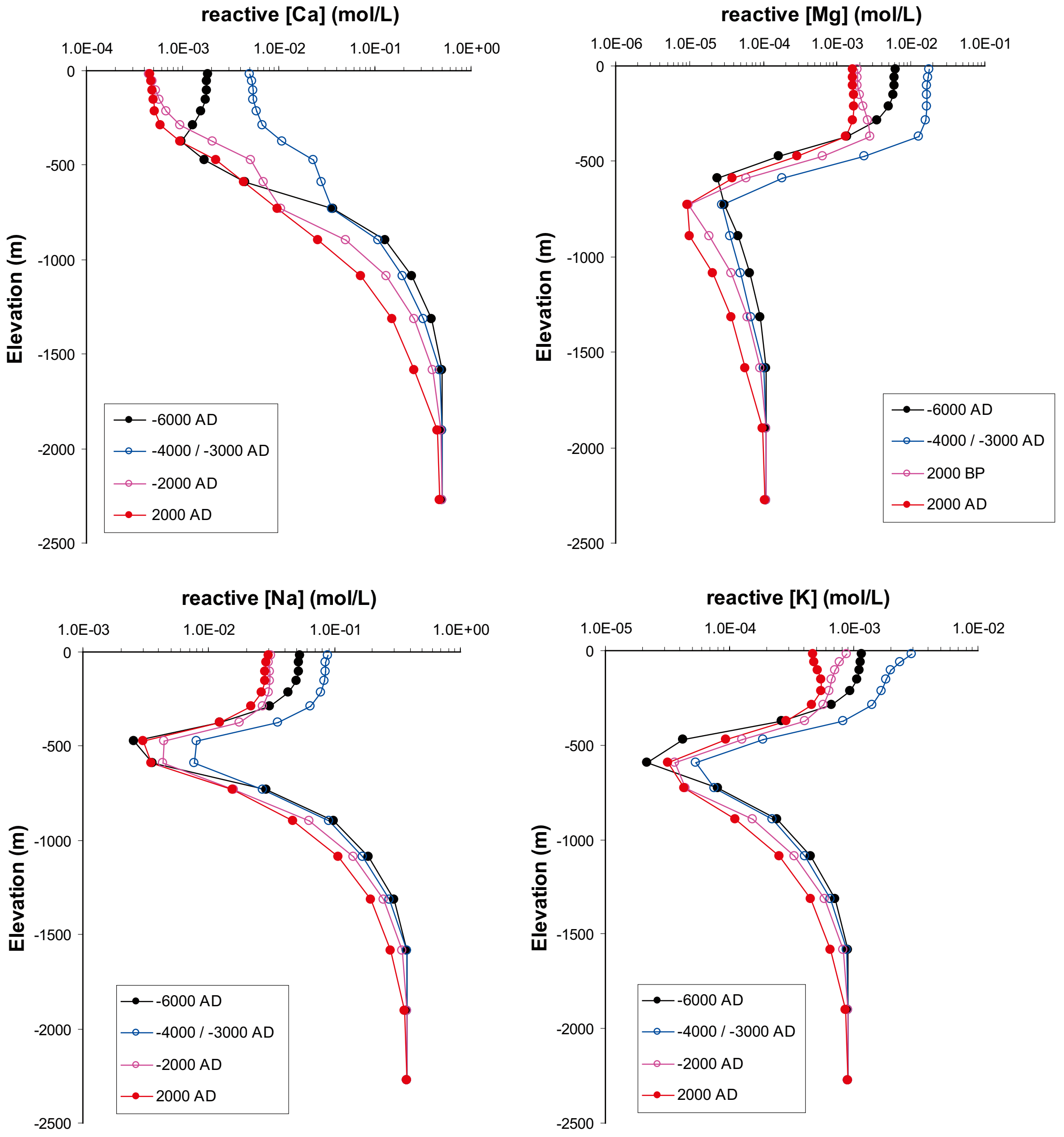

Figure 4-10. *Distribution of the reactive concentrations obtained, related to the depth (in the km 7 of the numerical model and crossing the EW007 fault zone).*

Chlorite dissolution and quartz and illite precipitation occur in the shallowest areas of the simulated domain, where the meteoric waters are directly interacting with rocks (Figure 4-11). As a qualitative indication, by every two volumetric units of dissolved chlorite, one volume of illite and three volumes of quartz are obtained.

Plagioclase (considered as a mineral phase of the matrix bedrock) dissolves along the walls of the fracture zone. Calcite dissolves above –300 m, and precipitates between –300 m and –1,000 m. At depths around –500 m, a maximum amount of calcite is precipitated, reactivating chlorite dissolution and illite precipitation. As a consequence of these reactions, and the combined effect of the descending fluid flow, the pH values decrease down to –500 m. In this way, kaolinite oversaturation is reached, precipitating accordingly with calcite precipitation.

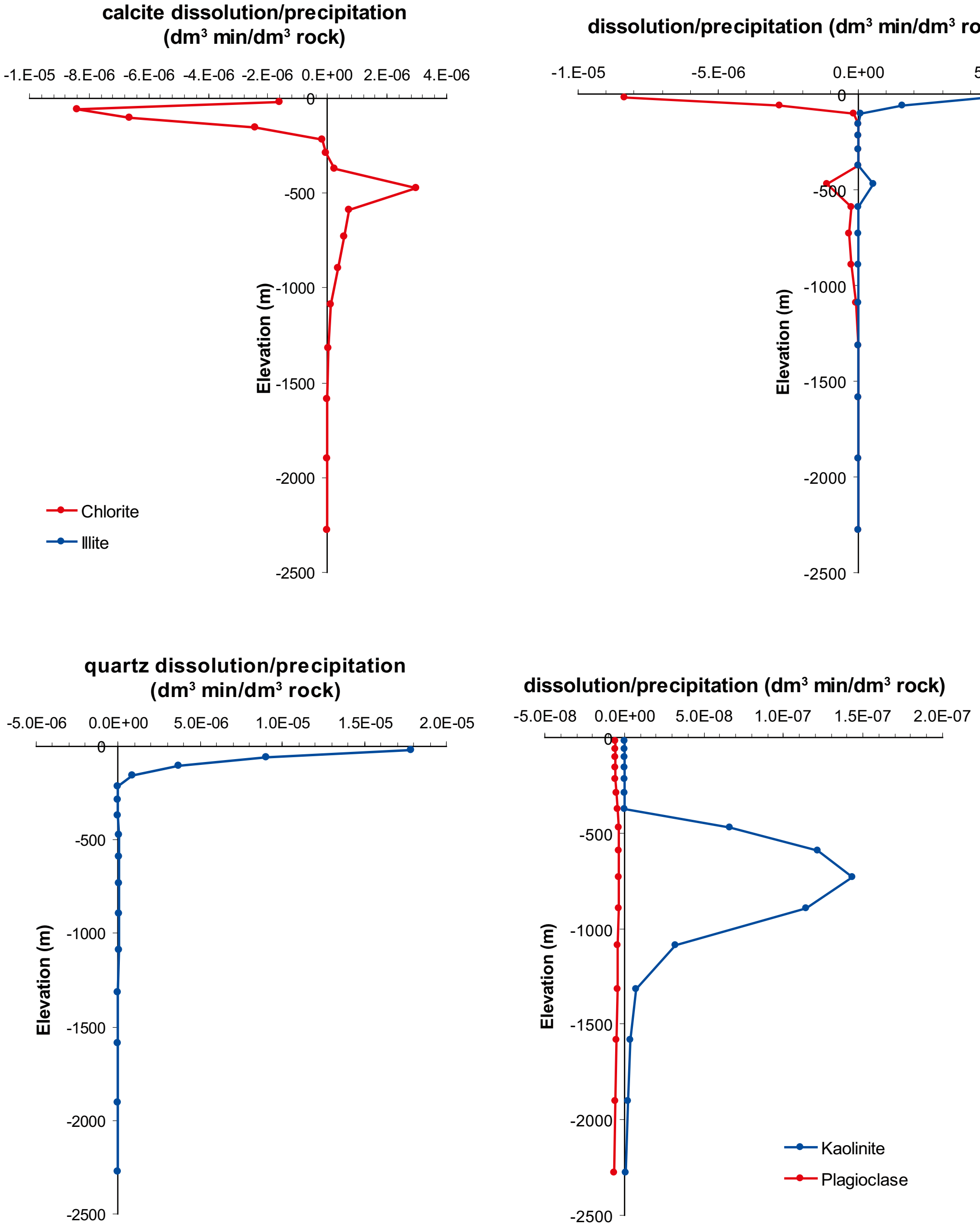

Figure 4-11. *Distribution of the cumulative volumes of the mineral dissolved (red line) or precipitated (blue line), related to the depth (2000 AD, in the km 7 of the numerical model and crossing the EW007 deformation zone).*

By comparing computed results of the reactive transport model and the non-reactive transport model, it can be observed that a deficit of calcium is registered in the shallowest groundwaters (Figure 4-12). This is a consequence of the uptake of calcium by the solid exchanger. In spite of calcite and plagioclase dissolution supplying calcium to the solution, it is removed of the groundwaters by the cation exchange reactions. In this way, calcite and plagioclase saturation decrease, progressing their dissolution.

During the period from 6000 until 3000 BC, the Littorina seawater infiltrated across to the upper boundary of the domain (Figure 4-1). The composition of this water is relatively enriched in magnesium and sodium (with respect to its calcium concentration; Table 3-1). Consequently, the aqueous species of magnesium and sodium were preferentially exchanged by the solid phases, which releases calcium to the groundwater. During the period from 3000 BC until 2000 AD, meteoric water becomes the most important contributior of the surface recharge. Meteoric water is enriched in calcium, which is being preferentially fixed in the solid exchanger, releasing magnesium and sodium to the groundwaters. Consequently, the simulated groundwater composition

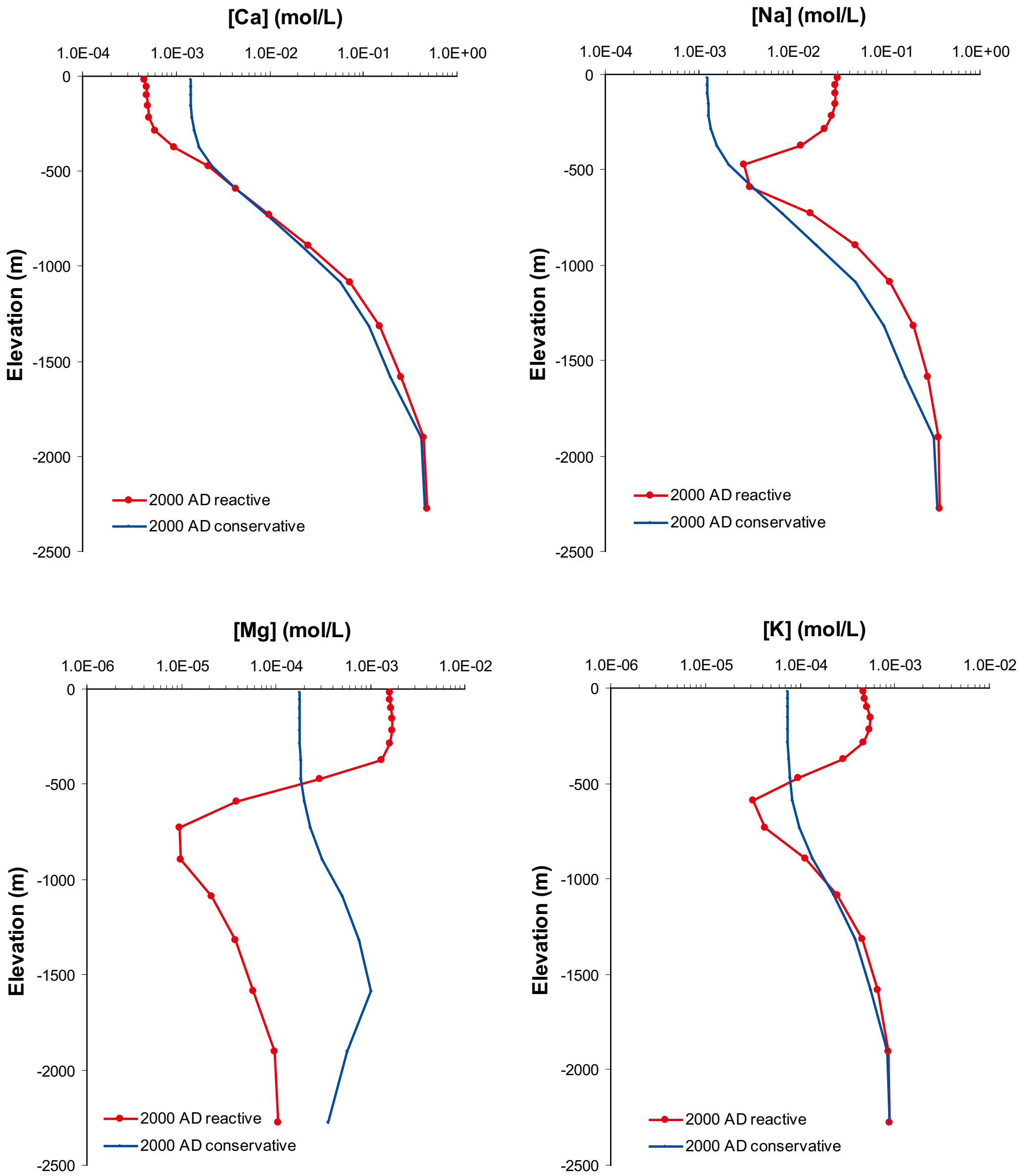

Figure 4-12. *Comparison between the computed concentrations obtained by the reactive and the conservative transport models (2000 AD, in the middle of the domainf the numerical model of the EW007 fault zone).*

above the –500 m, in the EW007 deformation zone, is characterised by a deficit of calcium and an excess of magnesium, sodium and potassium (with respect to the expected concentrations calculated by the conservative transport model; Figure 4-12).

Down to –500 m, groundwaters show a significant enrichment in sodium that was preferentially fixed in the solid exchanger in contact with the deep saline groundwater. When deep saline groundwaters are washed-out by the meteoric groundwaters, sodium sited in the solids are exchanged by cation aqueous species (e.g. magnesium), increasing the aqueous sodium concentration (Figure 4-12).

4.4 Evaluation of the influence of geochemical processes in the apparent Littorina signatures

Magnesium is present in the Littorina seawaters at much larger amounts than in the other reference waters. /Molinero et al. 2008/ analysed the empirical relaltionship between computed M3 Littorina mixing fractions and measured magnesium concentrations in Forsmark (Figure 4-13). The following empirical law was observed in the case of Forsmark:

$$\%\ \text{theoretical Littorina composition} = (0.0019\cdot[\text{Mg}]) + 0.0284 \qquad \text{Equation 4-1}$$

where [Mg] is the concentration of magnesium expressed in mg/L. However, it is well known that dissolved magnesium is a reactive species that can be involved in a number of hydrogeochemical processes, one of the most relevant being cation exchange. The work summarised here aims at evaluating the magnitude of the error that could be committed when magnesium is used as a conservative tracer for Littorina water.

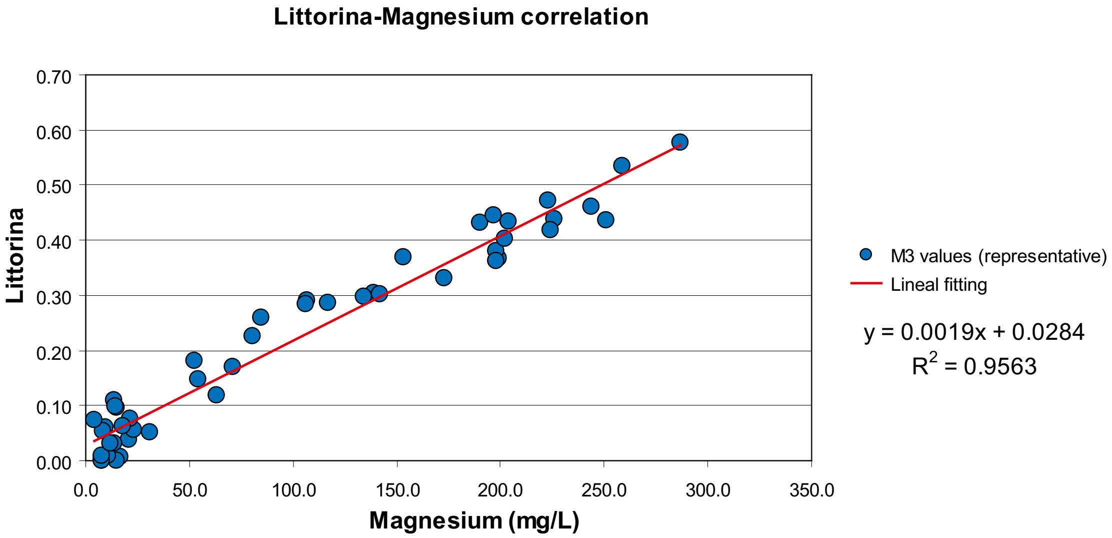

***Figure 4-13.** Correlation between Littorina mixing fractions and dissolved magnesium in groundwater samples from Forsmark.*

The theoretical proportion of Littorina seawater in the mixture has been calculated according to the reactive and the conservative magnesium concentrations (Figure 4-14). If the performed numerical models are regarded as a "synthetic reality", then the non-reactive amount of Littorina would be the "real Littorina signature" and the reactive transport simulations, considering cation exchenge processes, will give us the "apparent amount of Littorina signature" according to magnesium concentrations. According to model results, it can be seen that the "apparent" Littorina proportion obtained by the "synthetic reality" when using magnesium concentrations, is overestimated in the eastern (coastal area) and in the shallow parts of the domain, where the reactive magnesium concentrations are noticeably increased as a consequence of the cation exchange reactions (blue areas in the map of Figure 4-14). On the other hand, when the reactive magnesium concentrations are lower than the non-reactive values, the "apparent" amount of Littorina is underestimated by using magnesium (red areas in the map of Figure 4-14). Consequently, if the simulated reactive processes are similar to the actual processes happening in the site, then the amount of Littorina signatures computed by mixing models that use magnesium as a tracer would be similarly overestimated near the Baltic coast and underestimated at inland positions.

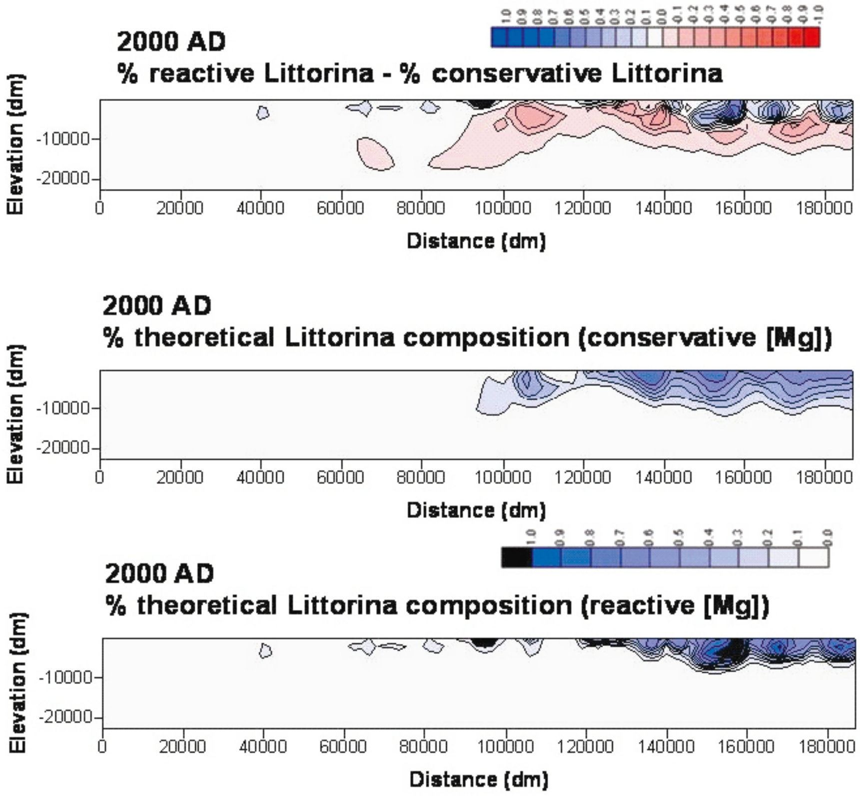

***Figure 4-14.** Comparison between the theoretical Littorina composition in the model by a conservative transport model (in the middle of the figure) and the "apparent" Littorina signatures by using the magnesium concentations computed in the reactive transport model (in the bottom of the figure). The upper figure corresponds to the difference between the "synthetic reality" (conservative Littorina tracer) and the "apparent" Littorina signature computed by reactive magnesium.*

4.5 Testing the reactive transport model with field measurements

Reactive transport model results have been tested by comparison with the available information from groundwater samples collected at boreholes located in the Laxemar subarea, near to the simulated cross section. Figure 4-15 shows computed and measured values of Cl^-, which can be regarded as a non-reactive species. The distribution of dissolved Cl^- is the result of the complex palaeohydrogeological history of the site. It can be seen that computed results reproduce relatively well the measured salinity distribution at depth. The observed agreement of Figure 4-15 is the confirmation of the good performance of the hydrogeologic models that supply flow fields and hydrodynamic parameters to the reactive transport simulations.

Figure 4-16 shows the comparison between (1) computed results of conservative transport simulations, (2) computed results of reactive transport simulations and measured values of Ca^{2+} and Na^+ concentrations. The role of geochemical processes in the groundwater composition can be evaluated by comparing measured data against conservative and reactive transport simulations. In this particular case (Figure 4-16) it can be seen that reactive transport processes produce a relative enrichment of Na^+ and depletion of Ca^{2+} in the groundwater. It can be seen that reactive transport simulations reproduce the measurements of reactive species in the Laxemar site, improving the results of the conservative transport simulatons. Differences between reactive and conservative solutes are more evident in the first 500 metres of the bedrock due to the influence of the more dynamic hydrogeologic system dominated by fresh waters of recent meteoric origin.

It can be seen in Figure 4-16 that computed results of the reactive transport model predicts a minimum value of dissolved Na^+ at about –500 m which is not seen in the field measurements. The same kind of minimum "peak" can be seen in other cations, such as Mg^{2+} (see Figure 4-17). Such behaviour of the model coincides with the assumed depth of maximum glacial waters initially present in the domain. The reactive transport model equilibrates the initial exchanger with the glacial waters and this fact has an influence on the computed results of the future. Thus, it can be stated that the reactive transport model shows a relevant sensitivity with respect to the uncertainty of the hydrochemical initial conditions, mainly related with the actual composition and location of the glacial melt waters infiltrated 8,000 years ago.

Figure 4-17 shows the comparison between (1) computed results of conservative transport simulations, (2) computed results of reactive transport simulations and measured values of Mg^{2+} and K^+ concentrations.

It can be seen that (Figure 4-17), in general, a non-reactive approach for magnesium underpredicts dissolved concentrations up to –700 m, and overpredict concentrations deeper than –700 m. It is worth noting that no calibration has been made in the reactive transport modelling, so computed results can be regarded as a pure prediction of the reactive species. Figure 4-17 indicates that some calibration of the reactive processes and parameters would be required to improve the model. Figure 4-17 also shows the computed values and field measurements of potassium. It can be observed that in this case, it seems that reactive processes affecting potassium are overestimated in the reactive transport model. In fact, computed results of the conservative transport model fit better the field measurements of potassium.

Figure 4-18 shows the comparison between (1) computed results of conservative transport simulations, (2) computed results of reactive transport simulations and measured values of HCO_3^- concentratioins and pH. These two variables can be regarded as two of the best reactive indicators in groundwaters. Figure 4-18 illustrates the ability of the numerical model to reproduce the reactive behaviour of the groundwater system and how computed results improve compared with the non-reactive solute transport model.

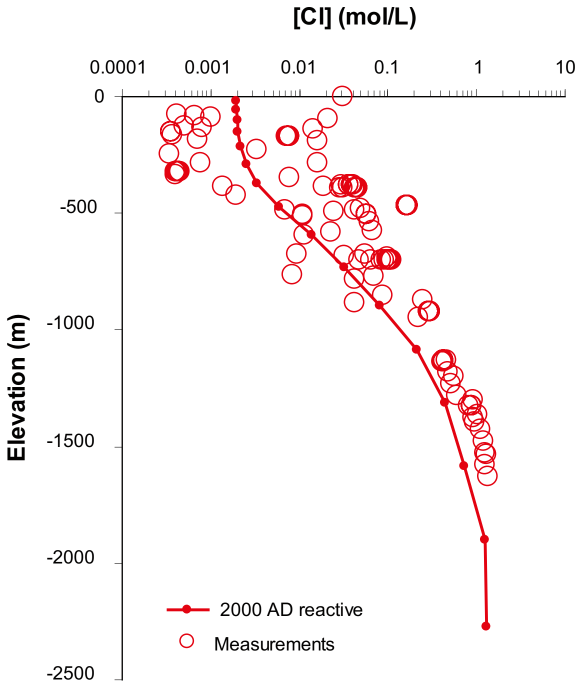

Figure 4-15. *Computed and measured concentrations of Cl^- (2000 AD) along a vertical profile located in the middle of the model domain.*

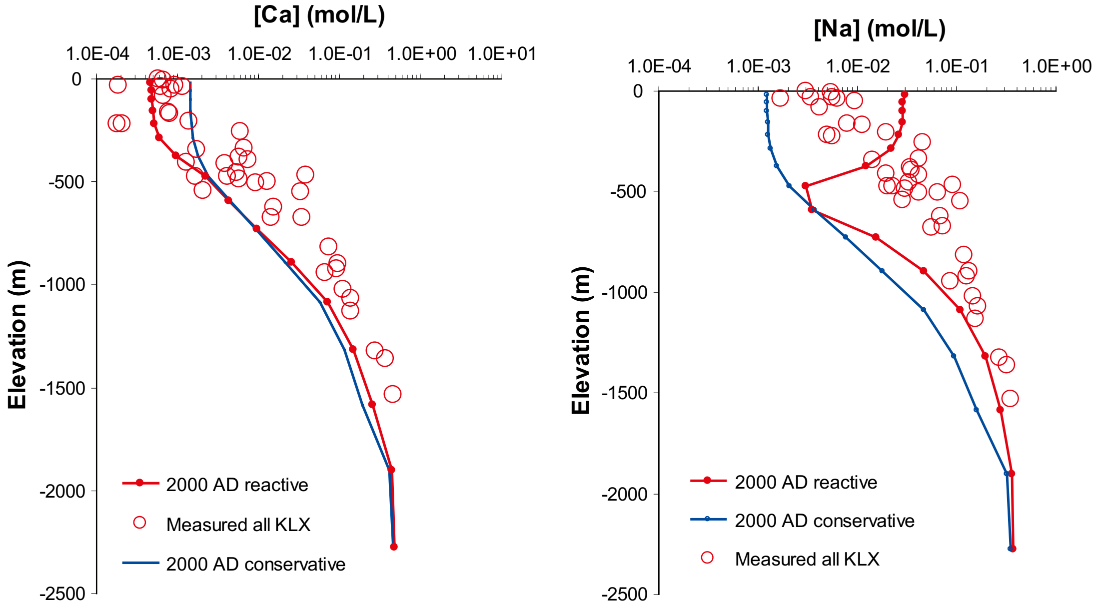

Figure 4-16. *Computed and measured concentrations of Ca^{2+} (left) and Na^+ (right) along a vertical profile located in the middle of the model domain. Computed results of a conservative transport run (blue) and a reactive transport run (red) are plotted to evaluate the influence of the geochemical processes on the dissolved concentrations.*

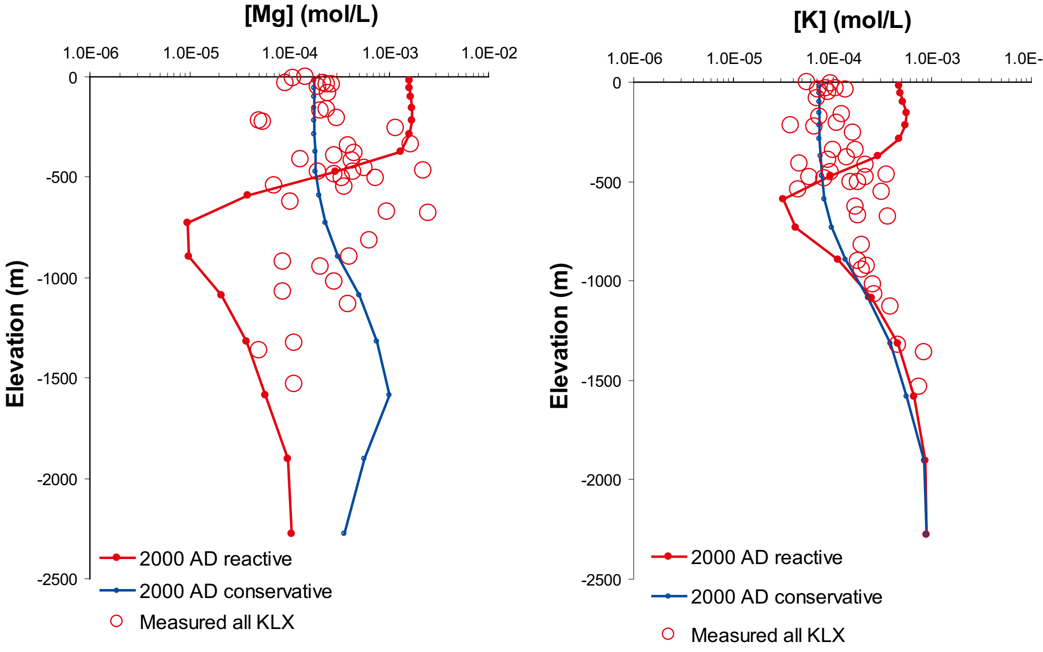

Figure 4-17. *Computed and measured concentrations of Mg^{2+} (left) and K^+ (right) along a vertical profile located in the middle of the model domain. Computed results of a conservative transport run (blue) and a reactive transport run (red) are plotted to evaluate the influence of the geochemical processes on the dissolved concentrations.*

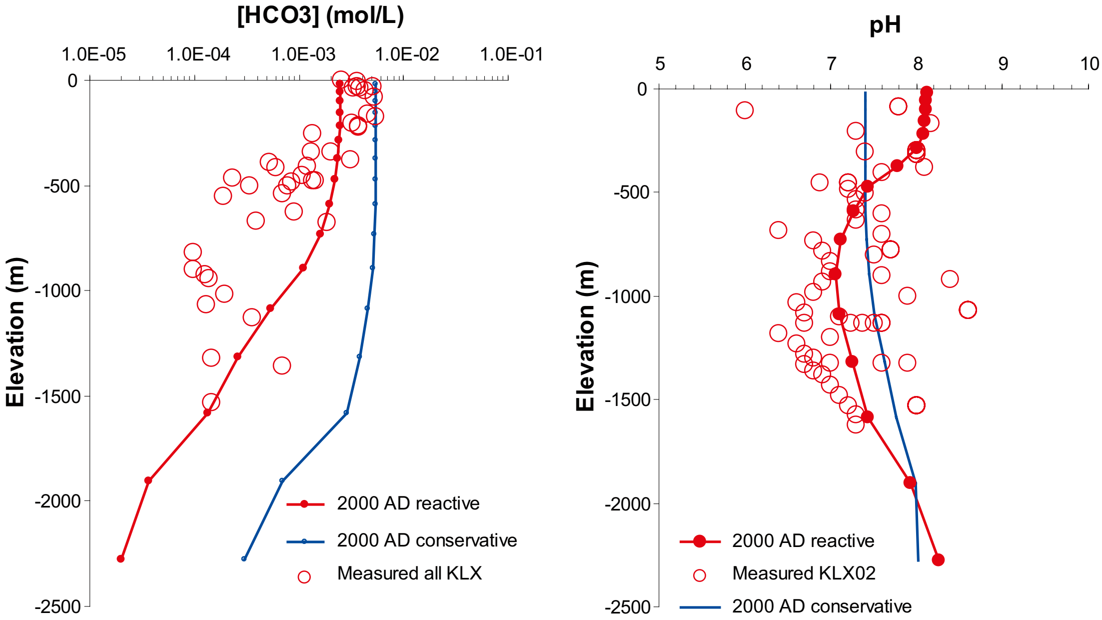

Figure 4-18. *Computed and measured concentrations of HCO_3^- (left) and pH (right) along a vertical profile located in the middle of the model domain. Computed results of a conservative transport run (blue) and a reactive transport run (red) are plotted to evaluate the influence of the geochemical processes on the dissolved concentrations.*

5 Conclusions

A methodology to simulate large-scale, long-term complex palaeohydrogeochemical evolution in fracture zones has been developed and compared with field data. The methodology integrates complex site-specific hydrogeologic models with geochemical reactive transport processes in two-dimensional domains. It is felt that this methodology constitutes a powerful tool to test and reinforce consistency and integration between hydrogeological and hydrogeochemical studies of the site. In addition, the reactive transport models developed here show great potential as a quantitative tool for understanding the hydrochemical conditions of the site, as well as possible changes under different future scenarios.

The hydrogeological problem is solved first, accounting for density-driven flow processes, with the hydrogeological, regional-scale, numerical model of the site (version 2.1). Then, computed flow fields are extracted at selected time periods and transferred to the reactive transport model. Then, the reactive transport simulator solves for a series of steady-state flow fields, updating such flow fields and boundary conditions in every simulated period. The hydrogeochemical results computed at the end of a given period are automatically used as inicial conditions for the next period.

A case-study has been simulated in the Laxemar site corresponding to a cross section that includes deformation zone EW007. The cross section runs parallel to the deformation zone and perpendicular to the coast line and the main topographic gradient. Then, it is thought that such a profile can be readily simplified with a two-dimensional flow field. The main geochemical processes identified in the geochemical conceptual model of the site have been considered in the simulations. It is worth noting that the current model do not incorporate redox sensitive processes.

Computed results show that numerical models can simulate the key geochemical systems influencing groundwater chemistry at the site: (a) calcite dissolution/precipitation, (b) silicates weathering and (c) cation exchange processes. A quasy steady-state calcite dissolution/precipitation front is computed at a depth between 100 and 250 m. Silicates initially present in the fracture fillingand the rock (i.e. plagioclase, K-feldspars and chlorite) are dissolved by infiltrating meteoric waters and, at the same time, clay minerals (i.e. illite and kaolinite) precipitate. It is also seen that cation exchange processes play a relevant role in some cations such as calcium, sodium and magnesium. The infiltration of Littorina waters produces an enrichment of magnesium in the solid exchanger. The subsequent infiltration of meteoric water, with lower contents of dissolved magnesium, produces a release of the magnesium previously fixed in the solid phase so that infiltrated meteoric waters are enriched in magnesium. This combined phenomenom can produce a kind of "memory effect" in the system that influence the Littorina signature, which is usually detected based on mixing models using magnesium as the main Littorina indicator.

Computed model results have been checked by comparison with measured concentration of major dissolved species at the Laxemar site. It is seen that reactive transport simulations can successfully reproduce most of the qualitative trends observed in the hydrochemical data of the major components. It is worth noting that the current modelling exercise has not been calibrated and/or adjusted to fit measured data. Thus, the current results can be seen as a quantitative integration exercise of the hydrogeological and hydrochemical conceptual models of the site. Computed results show that both conceptual models are sound and able to reproduce the major hydrogeochemical conditons of the Laxemar subarea. Further applications of the model could be done in order to make sensitivity analyses and include the redox sensitive processes.

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Section 3

Application of the Drilling Impact Study (DIS) to Laxemar groundwaters

Mel Gascoyne, GGP Inc
Ioana Gurban, 3D-Terra

Contents

1 Introduction

Characterisation of a geological formation as a repository for nuclear fuel waste requires deep drilling into the bedrock to gain an understanding of the geological structure, rock types, groundwater flow and the chemical composition of groundwater and the adjacent rock. The methods of characterisation from a hydrogeochemical point of view, might be affected by the various drilling activities and techniques for determining groundwater composition have been employed so that the composition can be corrected for these activities.

The Drilling Impact Study (DIS) project started in 2002 by SKB. A uranine tracer is mixed with drilling water to detect and quantify contamination and thereby allow correction of the groundwater composition for dilution or contamination by drill water. The project started about six years ago /Gurban and Laaksoharju 2002/ with the intention of developing a routine method for determining the extent of contamination of borehole groundwater by drilling water. The main objectives of the work were, 1) to determine the extent of drill water contamination in permeable zones in selected boreholes on the Forsmark site, 2) correct measured chemical compositions of the groundwaters based on contamination results, 3) provide a workable methodology for routine correction of groundwater composition, 4) apply the modified DIS model to suitable borehole zones at the Forsmark site in a systematic fashion and 5) determine uncertainties in DIS modelling.

2 Objectives of the DIS project

The aim of DIS is to investigate how the borehole drilling process affects groundwater composition. Clear limits are currently used to define how much drilling water is acceptable in a groundwater sample intended for chemical analysis. With increasing drill water content, the value of the sample is reduced for modelling purposes and the sample may even be discarded in the modelling. High drill water content is used in determining the categorisation of the samples and for planning of further sampling.

An important question in DIS that must be addressed is "do we understand the process of disturbance caused by drilling water"? The answer is currently "no". To improve this situation we need to study the impact of drilling water on parameters such as the redox sensitive elements and the effect of dissolution major components in groundwater more carefully.

For example, Figure 2-1 shows a plot of Fe^{2+} in groundwater versus drill water content for Laxemar 2.3 /Laaksoharju et al. 2009/. The expectation is that increased drill water content oxidises iron and hence decreases the Fe^{2+} content. This appears not to be the case, however, because in Figure 2-1, the iron content can be either low or high for a given level of drill water. This be due to the presence of oxygen in the drill water, microbial processes, redox buffer capacity of the bedrock or mixing.

It is hoped that the DIS study for Laxemar could try to answer the above anomalies and questions and should therefore include:

1) **Response evaluation:** Detailed evaluation of samples from repository depth in order to study the behaviour of redox sensitive elements and major components.
2) **Response modelling:** Modelling time-series data where the injection of drill water is modelled and where the modelled values are compared with measured data.
3) **Sensitivity analysis:** How much drilling water can be injected (data and modelling) before the sample becomes worthless (i.e. when the sample is dominated by drilling water).
4) **Evaluation:** How can samples with high drill water content be used for modelling?

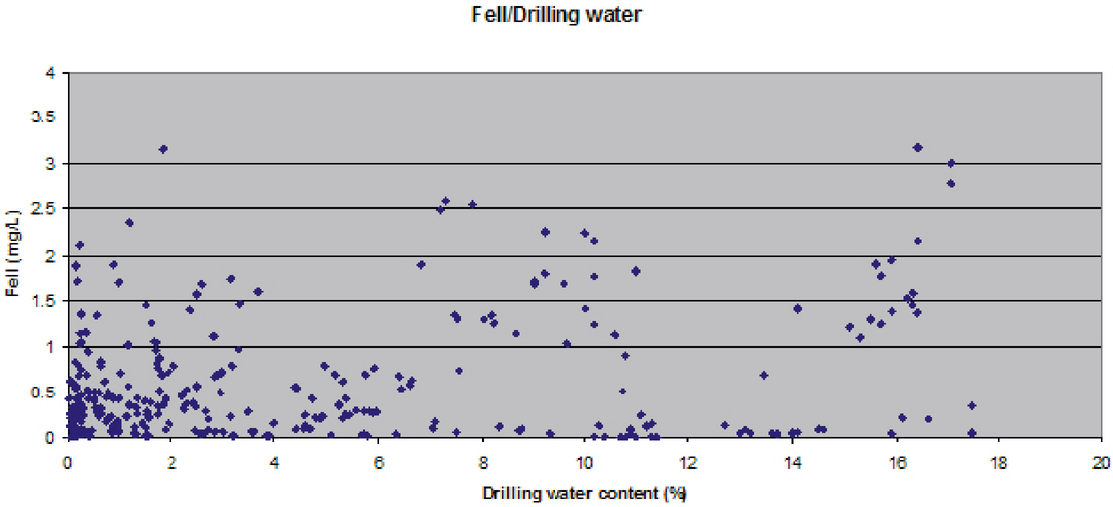


Figure 2-1. *Fe^{2+} concentration and drill water content for Laxemar boreholes, drill water return.*

3 Drilling water and tracer concentrations used in Laxemar boreholes

A summary of the hydrogeological and pumping/injection history of Laxemar boreholes and their permeable zones, made during the drilling period, is given in Table 3-1 based on information from the site records. Indication is given in this table as to whether the permeable zone is suitable for DIS testing, based on the five criteria: a) reliable measurements of uranine in drilling return water, b) stability of uranine injection and satisfactory recording of data, c) adequate drill-water information (times, dates, rates, chemistry), d) adequate records of drilling water pumped in and out from the borehole during drilling, in time and along the boreholes length and e) presence and adequacy of chemical analyses of groundwater.

3.1 Borehole information

Of the 14 Laxemar boreholes potentially suitable for applying DIS techniques (Table 3-1) only 5 gave adequate monitoring data that would permit DIS calculations. These are packer-isolated sections in boreholes KLX03, KLX08, KLX13A, KLX15A and KLX17A (indicated in Table 3-1). The criteria for selecting these boreholes were:

1) Sections at repository depth (300–700 m depth); exception was made for one section at –922.45 m depth in KLX03.
2) Sections with time series (more than 3 samples).

Criteria for rejection include:

1) Sections with severe short-circuiting of flow past packers or through interconnecting fractures.
2) Monitoring sections.
3) Old boreholes (e.g. KLX01 and KLX02).

Table 3-1. Details of the KLX (Laxemar) borehole sections and their suitability for application of DIS (data provided/obtained from the Extended data freeze Laxemar table from data provided by /Gimeno et al. 2009/ and /Laaksoharju et al. 2009/.

IDCODE	Elevation SecMid	SECUP (m)	SECLOW (m)	Comments	DIS calculations
KLX01	–163.26	171.00	190.00	old borehole	no
KLX01	–257.06	272.00	277.00	old borehole	no
KLX01	–440.73	456.00	461.00	old borehole	no
KLX01	–672.95	680.00	702.11	old borehole	no
KLX01	–817.20	830.00	841.00	old borehole	no
KLX01	–897.09	910.00	921.00	old borehole	no
KLX01	–1,019.91	999.00	1,077.99	old borehole	no
KLX02	–298.57	315.00	321.50	old borehole	no
KLX02	–318.13	335.00	340.80	old borehole	no
KLX02	–452.50	452.00	494.00	old borehole	no
KLX02	–778.18	798.00	803.80	old borehole	no
KLX02	–1,068.24	1,090.00	1,096.20	old borehole	no
KLX02	–1,129.14	1,145.00	1,164.00	old borehole	no
KLX02	–1,134.60	1,155.00	1,165.00	old borehole	no
KLX02	–1,322.81	1,345.00	1,355.00	old borehole	no
KLX02	–1,530.98	1,420.00	1,700.50	old borehole	no
KLX03	–170.82	193.50	198.37	shallow section	no
KLX03	–379.85	408.00	415.30	Cat 3, possible instability, borehole used later for tracer tests	yes
KLX03	–700.60	735.50	748.04	Cat 5, unstable, possible short–circuiting, borehole used later for tracer tests	yes
KLX03	–922.45	964.50	975.15	Cat 1, should be very good, borehole used later for tracer tests	yes
KLX05	–204.84	241.00	255.00	shallow section	no
KLX06	–221.18	256.00	275.00	shallow section	no
KLX06	–475.27	554.00	570.00	only 2 samples	no
KLX07A	–569.69	753.00	780.00	Cat 5, monitoring section! Short-circuiting + monitoring	no
KLX08	–150.43	197.00	206.65	shallow section	no
KLX08	–320.03	396.00	400.87	Cat 5 short circuiting between section and the upper bedrock hosting young meteoric recharge groundwater	yes
KLX08	–390.73	476.00	485.65	Cat 2 Should be OK	yes
KLX08	–504.54	609.00	618.51	Cat 3 possible short-circuiting	yes
KLX10	–31.78	0.00	100.60	shallow section	no
KLX10	–338.43	351.00	368.00	only 2 samples	no
KLX10	–676.19	689.00	710.00	only 2 samples	no
KLX11A	–465.97	516.50	519.50	only 2 samples	no
KLX12A	–501.12	535.00	545.00	only 2 samples	no
KLX13A	–408.01	432.00	439.16	Cat 3 possible instability	yes
KLX13A	–474.99	499.50	506.66	Cat 4 possible short-circuiting	yes
KLX15A	–467.22	623.00	634.51	Cat 2 Should be OK	yes
KLX17A	–342.32	416.00	437.51	Cat 3, possible instability	yes
KLX17A	–547.97	642.00	701.08	Cat 5 Severe short- circuiting	no
KLX19A	–413.86	509.00	517.00	Cat 3, monitoring section!	no

Cat = Groundwater sample Category.

In a previous Forsmark study, /Gascoyne and Gurban 2008/, one borehole (KFM06A) was used as the test case for application of DIS. Detailed records of drill water injection, withdrawal and tracer volumes and concentrations were made. All data used were selected from the SKB database Sicada and, where available, reports of these measurements and characteristics of the drilling were obtained from borehole-specific reports such as that of /Berg et al. 2005, 2006/.

In the Laxemar study, however, volumetric data for drill water injection ('flushing') water for 3 boreholes (KLX03, KLX08 and KLX13A) were not initially available at the time of preparation of this report and so full application of DIS was not possible until just recently. The data selected in the Laxemar study showed that borehole drilling took place over the period 2004–2007. The variations with depth of uranine concentrations in the drill waters for the five boreholes are shown in Figures 3-1 to 3-5 inclusive. These diagrams show that uranine concentrations lie close to the planned injected levels (~ 0.20 mg/L) and none of these waters showed evidence of a trend to lower or higher concentration over the period of drilling (such as might be caused, for instance, by a malfunctioning pump or analytical error).

Borehole KLX13A shows a trend of decreasing uranine in the return water, from 0.2 mg/L to < 0.05 mg/L, over the first 500 m of drilling. Borehole KLX08 shows an even more distinctive trend, reducing from 0.2 mg/L at 200 m to < 0.05 mg/l by 500 m and decreasing further, to ~ 0.01 mg/L for the remainder of the borehole.

Uranine concentrations in the return water were generally lower (~ 0.05 to 0.15 mg/L) than in injected levels, indicating loss of tracer to the fracture system and/or dilution by formation groundwater.

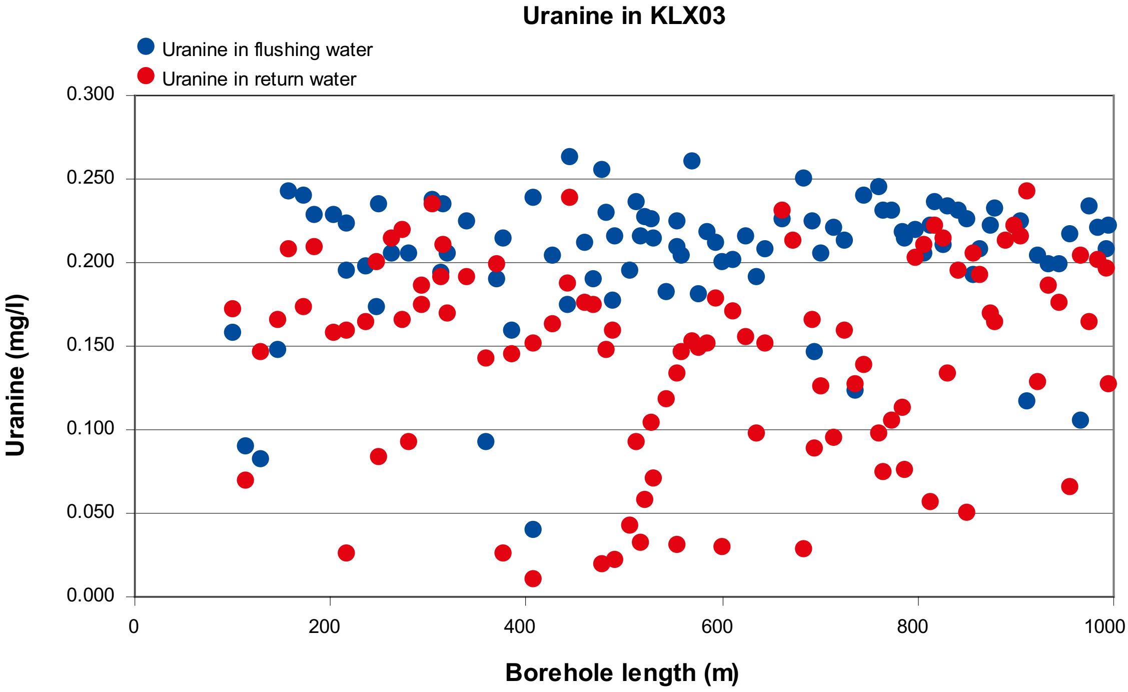


***Figure 3-1.** The variation of uranine concentrations in the drill water in KLX03.*

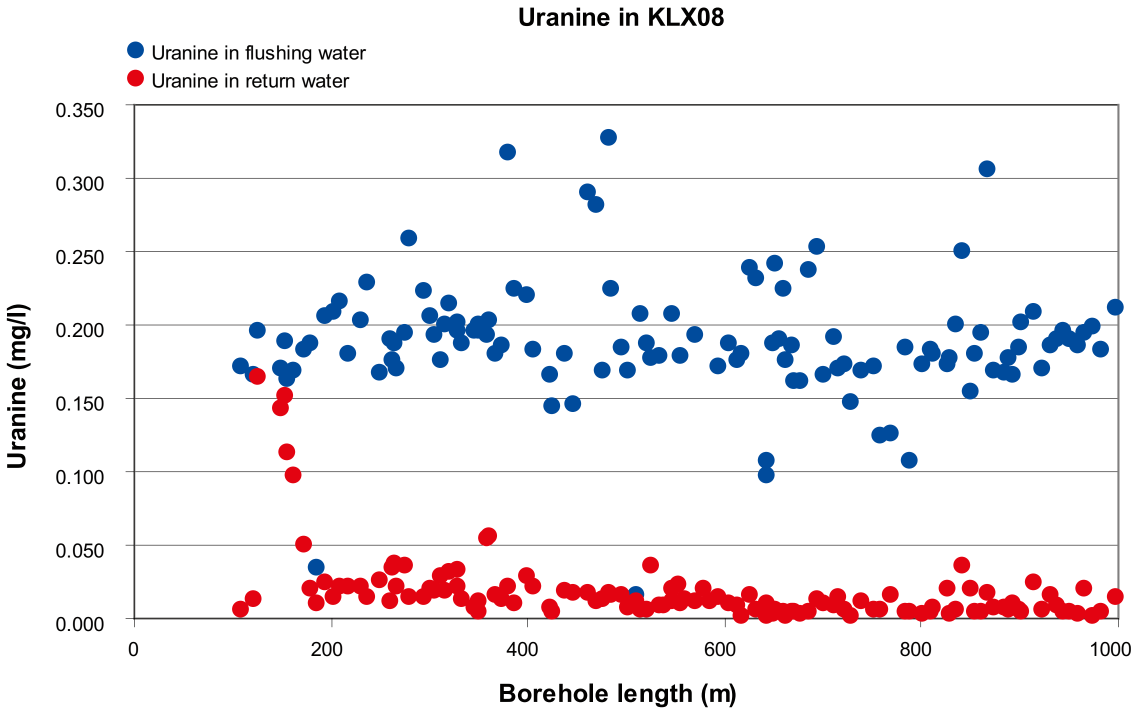


Figure 3-2. *The variation of uranine concentrations in the drill water in KLX08.*

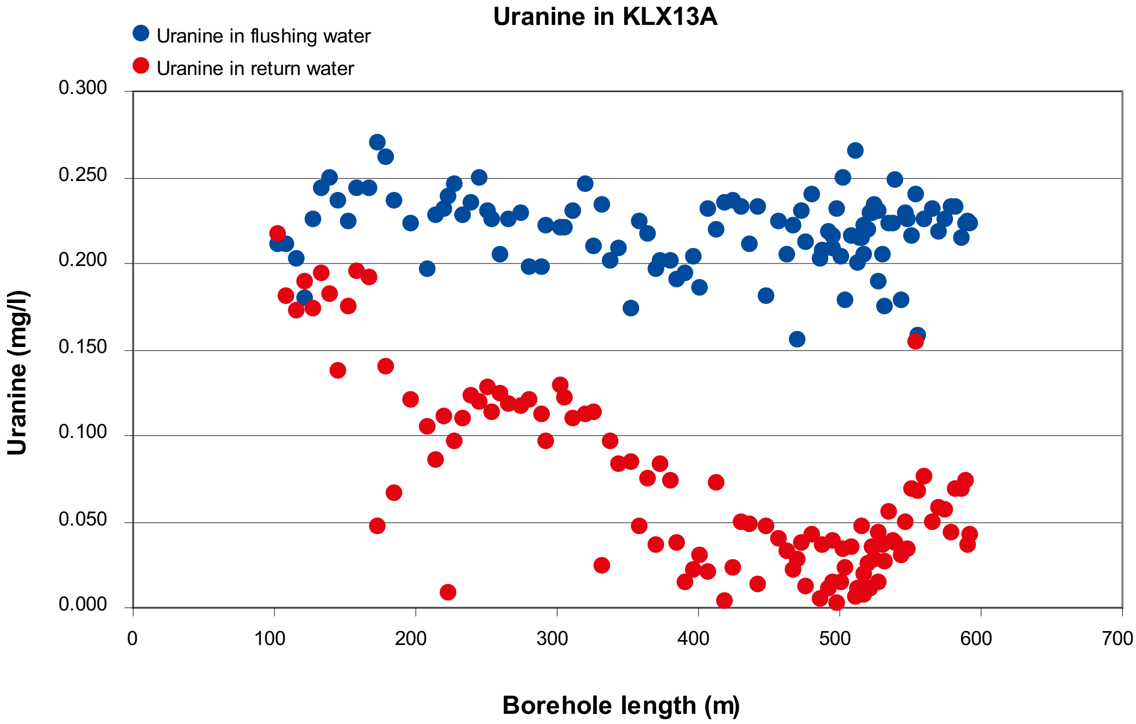


Figure 3-3. *The variation of uranine concentrations in the drill water in KLX13A.*

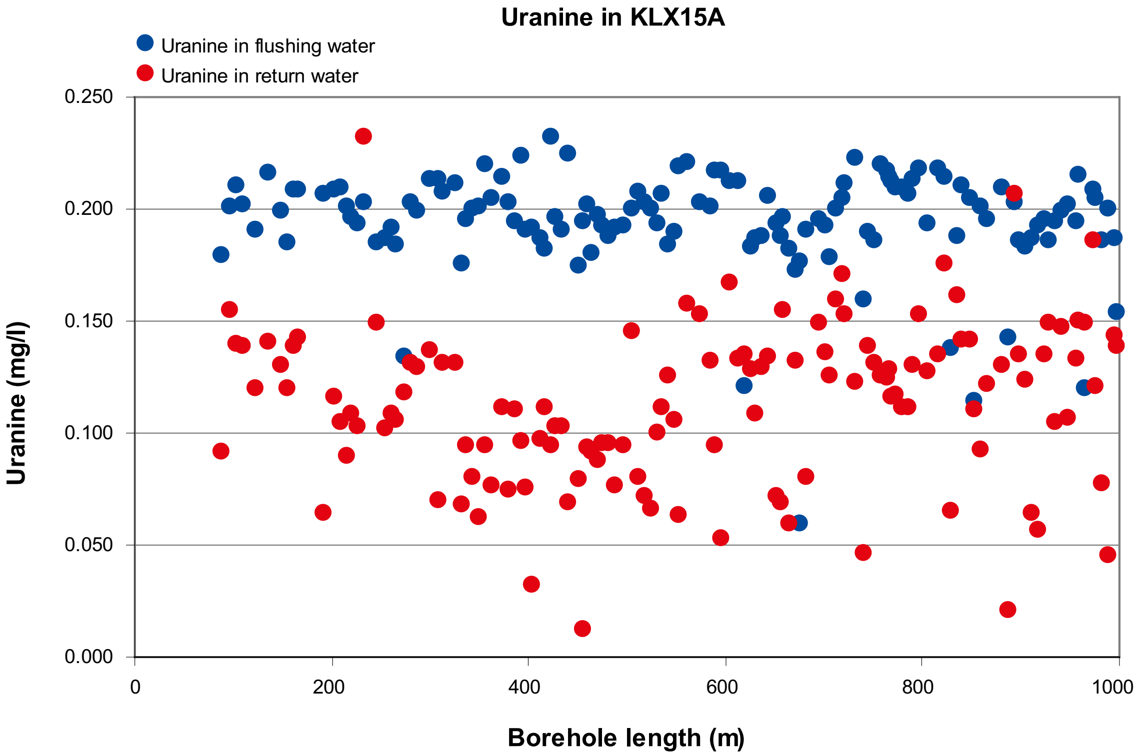


***Figure 3-4.** The variation of uranine concentrations in the drill water in KLX15A.*

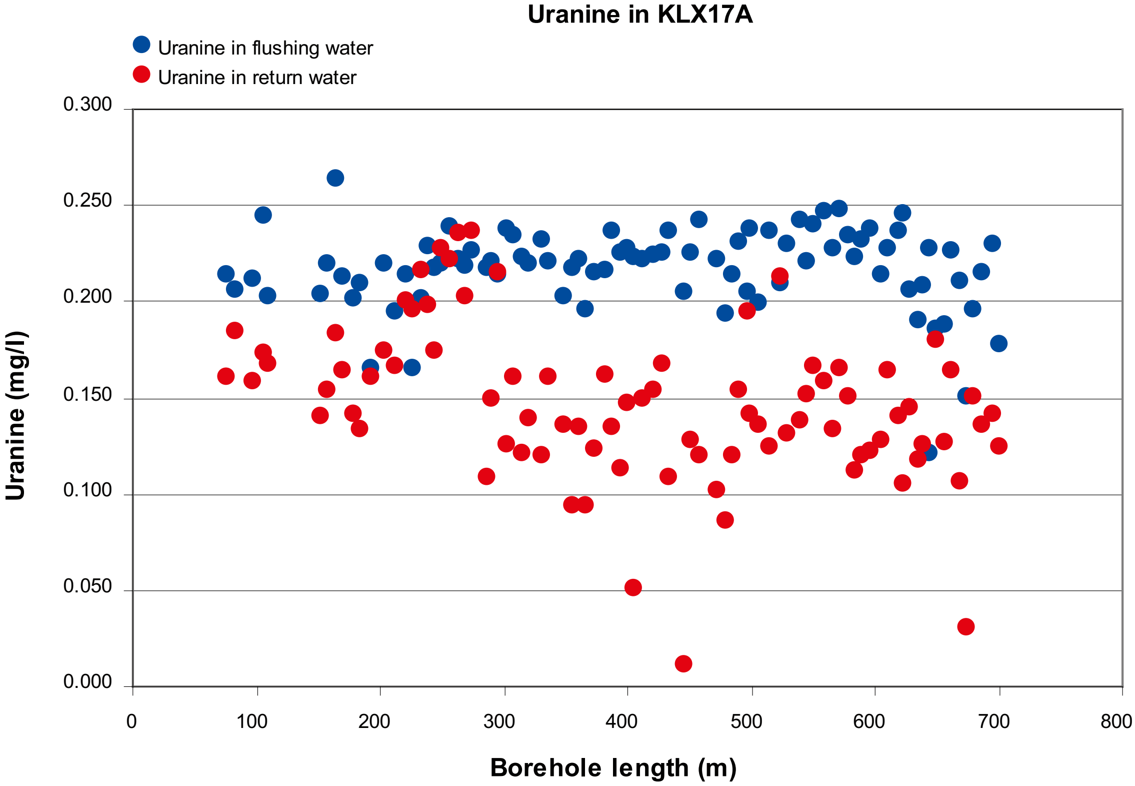


***Figure 3-5.** The variation of uranine concentrations in the drill water in KLX17A.*

3.2 Calculation of drill water content

The main aims of DIS are to evaluate the extent of contamination of individual fracture-zone groundwaters due to drilling activities, and then to determine how much groundwater must be pumped from each zone to reduce the uranine content to an acceptable level. The results of this modelling are then compared with the hydrochemical data obtained from each zone. The variation of cumulative injected and withdrawn drilling waters for each borehole are shown in figures in Appendix 1.

3.2.1 Basic calculations

The average content of uranine in borehole groundwater at the end of the drilling can be calculated in two ways, as follows (after /Berg et al. 2005, Gurban and Laaksoharju 2002/).

1. Gravimetric:

   Weight of uranine added to injected drill water (from gravimetric measurement).

   Weight of uranine returned to surface in return drill water (from weighted means).

   Average content of drill water in borehole groundwater.

2. Volumetric:

   Volume of drill water injected (from meter).

   Volume of drill water return (from meter; this represents drill water mixed with formation water).

The gravimetric method is more accurate because uranine weights are more precisely determined than are the water volumes.

3.2.2 Calculation of drilling water content in section groundwaters

An estimation of the uranine left in sections during drilling can be made from the uranine concentration in drilling and return water records. This is at best a rough estimation from the uranine values. This estimate could be compared to what was found in the sections after pumping and before or during sampling. Initially, the flushing volumes were not available and it was not possible to calculate the drilling water volumes left in the fractures during drilling. Only the uranine % could be determined. This gave a rough estimation of the extent of contamination of each section and served as a guide to later calculations. The Table 3-1 of (Nilsson, section # 4, this report) presents the average uranine per borehole. In Table 4-1 are calculated the uranine concentrations in the flushing water and return water when drilling each investigated section.

During slow-pumping for sampling purposes, the volume of water removed from the borehole zones is measured and, from the drilling records, the accumulated drilling volumes, in and out, can be calculated. Based on these calculations, the maximum amount of drilling water lost in the fractures during drilling can be determined. In all the cases (Appendix 1) the volume of return water exceeds that of flushing water.

Based on the uranine content in the return water, the volume of return water could be recalculated (Table 5-1). However, even if corrected, the return water exceeds the flushing water in five sections. This is probably due to extra pumping during drilling. For the five sections where the flushing volume remaining in the fractures could be calculated (KLX08, KLX15A and KLX17A), the results can be compared with the records of volumes removed during sampling. The residual volumes in the fracture systems after drilling calculated are then compared with the volumes pumped during sampling and the % of drilling water sampled. This helps to calculate what volumes should have been removed from the sections in order to eliminate the drilling water.

The basic calculations can be applied to the Laxemar data, however, and the results of this are given in Tables 3-2 to 3-6, below (based on data in the cited P- reports).

Table 3-2. (Table 5-14 from P-05-167).

Balance calculation of uranine tracer in KLX03.

Average uranine content IN (mg/L)	0.20
Volume IN (m³)	1,000
Amount uranine introduced (g)	200
Average uranine content OUT (mg/L)	0.14
Volume OUT (m³)	1,200
Amount uranine recovered (g)	170

Table 3-3. (Table 5-18 from P-06-222).

Balance calculation of uranine tracer in KLX08.

Average uranine content IN (mg/L)	0.183*
Flushing water volume IN (m³)	1,000
Amount uranine introduced (g)	183
Average uranine content OUT (mg/L)	0.019
Return water volume OUT (m³)	2,600
Amount uranine recovered (g)	49

* Uranine content based on results from Äspö laboratory.

Table 3-4. (Table 5-16 from P-07-195).

Balance calculation of uranine tracer in KLX13A.

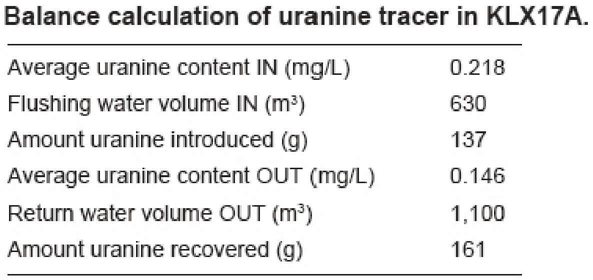
	Assuming that the DMS return water flow is correct	Assuming that the amount of uranine should be in perfect balance
Average uranine content IN (mg/L)	0.219	0.219
Flushing water volume IN (m³)	800	800
Amount uranine introduced (g)	175	175
Average uranine content OUT (mg/L)	0.070	0.070
Return water volume OUT (m³)	4,000	2,500
Amount uranine recovered (g)	280	175

Table 3-5.

Balance calculation of uranine tracer in KLX15A.

Average uranine content IN (mg/L)	**0.196**
Flushing water volume IN (m³)	**1100**
Amount uranine introduced (g)	**216**
Average uranine content OUT (mg/L)	**0.113**
Return water volume OUT (m³)	**1780**
Amount uranine recovered (g)	**201**

Table 3-6. (Table 5-15 from P-07-221).



Balance calculation of uranine tracer in KLX17A.

Average uranine content IN (mg/L)	0.218
Flushing water volume IN (m^3)	630
Amount uranine introduced (g)	137
Average uranine content OUT (mg/L)	0.146
Return water volume OUT (m^3)	1,100
Amount uranine recovered (g)	161

4 Hydrochemical sampling and analytical results

4.1 Sampling criteria

Groundwaters from the selected boreholes are defined as SKB chemical types and so several precautions were taken to minimise contamination by the drill water:

1. The drilling water supply well should also be of a SKB chemical type.
2. Boreholes HLX10 and HLX14 were selected to supply drilling and flushing water for the boreholes because of the acceptable concentration of total organic carbon (2.9 to 5.8 for HLX10 and 7.8 for HLX14) mg/L, target < 10.0 mg/L).
3. Dosing equipment for uranine was used instead of a storage tank (the latter may suffer from biological activity).

4.2 Drill water compositions

Drilling of the Laxemar boreholes was performed using water from the adjacent shallow percussion boreholes HLX10 (for KLX08) and HLX14 (for KLX03, KLX13A, KLX15A and KLX17A) as drilling fluid. This water is fresh in composition (Na-HCO_3 dominated) but somewhat more saline than surface waters or shallow groundwaters (see compositions at the end of Appendix 2).

4.3 Groundwater compositions

The compositions of groundwaters from each of the sections are listed in the table of data in Appendix 2. These data are plotted in figures showing major and minor ion concentrations against date of sampling in Appendix 3 and against percent of residual drill water in Appendix 4.

The characteristics of groundwater from each of the sections during drill water return pumping are summarized in Table 4-2. It can be readily seen that the expected trend (increase in ion concentration with decrease in percent of drill water) rarely occurs. These data are shown graphically in Appendix 4. Despite the lack of expected.

The characteristics of each of the sections during drill water return pumping are summarized in Table 4-2. It can be readily seen that the expected trend (increase in ion concentration with decrease in percent of drill water) rarely occurs. These data are shown graphically in Appendix 4. Despite the lack of expected relationships in Table 4-1, it is clear that the major components (Cl, Na, Ca, SO_4) all follow similar trends and HCO_3 appears to follow an inverse trend, as might be expected.

Table 4-1. Estimation of the uranine % left in the flushing water during drilling of the investigated sections.

ID CODE	SEC UP (m)	SEC LOW (m)	Uranine in drilling water (mg/l)	Uranine in return water (mg/l)	Sample nr (during drilling)	Uranine drill water - Uranine return water (mg/l)	% uranine left in section with the drilling water	Chemical sampling	
								COMMENTS	Drilling water residue (%)
KLX03	408	415.3	0.2386	0.1516	S/R 28	0.087	36	Cat 3	3.3
KLX03	735.5	748.04	0.2394	0.1379	S/R 66	0.1015	42	Cat 5	6.83
KLX03	964.5	975.15	0.23272	0.1636	S/R 93	0.06912	30	Cat 1	0.15
KLX08	396	400.87	0.2196	0.0286	S/R 42	0.191	87	Cat 5	0.86
KLX08	476	485.65	0.225	0.0155	S/R 52	0.2095	93	Cat 2	20.2
KLX08	609	618.51	0.1796	0.0021	S/R 72	0.1775	99	Cat 3	10.9
KLX13A	432	439.16	0.2113	0.0477	S/R 55	0.1636	77	Cat 3	11.3
KLX13A	499.5	506.66	0.2497	0.0337	S/R 72	0.216	87	Cat 4	14.1
KLX15A	623	634.51	0.1865	0.1085	S/R 74	0.078	42	Cat 2	7.55
KLX17A	416	437.51	0.2362	0.1092	S/R 47	0.127	54	Cat 3	1.18

Table 4-2. Characteristics of each of the sampled sections during pumping after drilling has ceased.

Borehole section	Characteristics
KLX 03-379	Concentrations stable, % residual slightly variable (no trend)
03-700	Concentrations increase as % residual increases
03-922	Concentrations stable as % residual slightly decreases
KLX 08-320	Concentrations stable as % residual slightly increases
08-390.73 (part 1)	High %, no trend (only 2 samples)
08-390.71 (part 2)	Concentrations stable, % residual slightly variable (no trend)
08-504	Concentrations stable as % residual is slightly variable (no trend)
KLX 13A-408	Concentrations slightly decrease as % residual decreases
13A-474	Concentrations slightly increase, % residual slightly variable
KLX 15A-467	Concentrations increase as % residual decreases
KLX 17A-342	Concentrations increase as % residual increases

The data shown in Appendix 2, for the major components (Na, Ca. Cl), indicate that, unlike the Forsmark site, some of the groundwaters show trends in the concentrations as described in Table 4-2.

The profile of Fe species varies considerably, in some cases showing a decrease in Fe^{2+} as % tracer is reduced (Figures KLX03-700, KLX13A-408 and 474, KLX17A-342), or an increase in Fe^{2+} (KLX03-379, KLX08-320, KLX08-504KLX15-467). The use of a relatively dilute drill water in KLX08 borehole (see bottom of table in Appendix 2, drill water chemistry), would tend to amplify the effect of contamination by drill water and would account for the greater variability of the major ion concentrations in the Laxemar site.

These data may be influenced, however, by the possible presence of uranine-tagged test water that was used in at least one Laxemar borehole (KLX03) as part of the Borehole Probe Dilution Test programme. In this programme, uranine (1 mg/L) was injected into packed-off borehole sections and allowed to disperse under natural gradients. Its concentration was followed by monitoring the dispersion into the fractures. This uranine was not pumped out at the end of the programme and so may account for some of the drilling water tracer that was subsequently measured.

5 Interpretation of DIS results

The plots showing the accumulated flushing and return water in the boreholes during drilling are presented in Appendix 1. As an example, the accumulated flushing and return water for KLX03 is presented here in Figure 5-1.

The drilling water volumes that may have been lost to host rock fractures in sections during drilling are presented in Table 5-1. In general, as shown in the graphs, the water volume withdrawn is higher than the water injected, meaning that the drilling water is mixed with formation water. Based on the average uranine data, approximate corrections of the return water were made (i.e. how much of the return water is in fact drilling water). Then the difference between flushing water and return water represents the flushing water left in the fractures. This calculation is possible only for KLX08 and KLX17. For the other boreholes, the difference is negative.

The simple calculations for uranine in flushing and drill-return water apply to the entire borehole, irrespective of the number, location and transmissivity of fractures intersected. When drilling has ended, it is important that a system of packers is installed as soon as possible to prevent cross-flow between permeable fractures at different depths. When first pumped for groundwater sampling, fractures that took drill water will initially yield groundwater that has a composition similar to drill water and most of the ambient groundwater will have been pushed back into the fracture system, driven by the pressure in the drill stem).

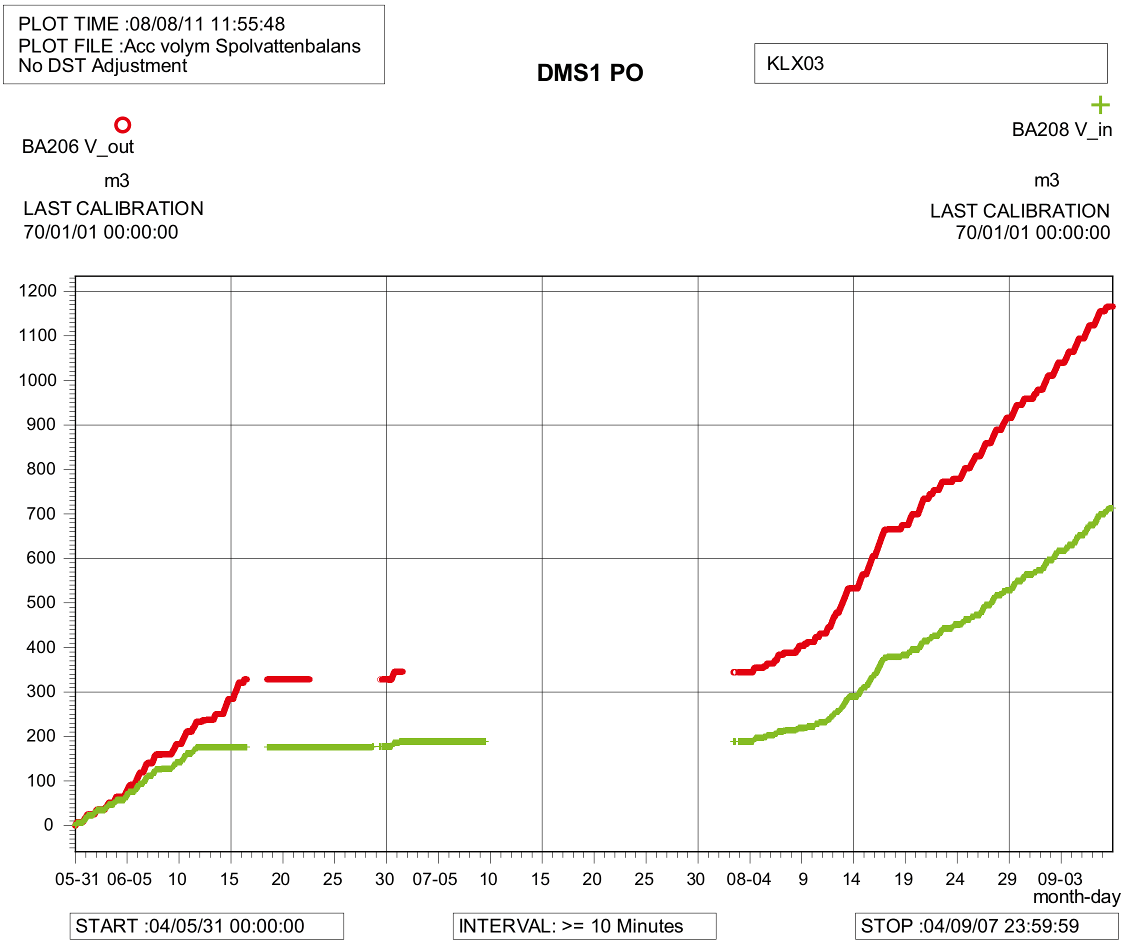


Figure 5-1. *KLX03 Plot Accumulated volumes flushing and returned water (plot obtained from Sicada and DMS databases).*

Table 5-1. Calculations of drilling water lost to fractures in the host rock based on uranine concentrations.

IDCODE	Elevation SecMid	SECUP (m)	SECLOW (m)	Water in (m3)	Water out (m3)	Average uranine return water	Water out corrected (m3)	Drilling water left in section (m3)
KLX03	–379.85	408	415.3	0	5.45	70%	3.82	-3.82
KLX03	–700.60	735.5	748.04	14.38	20.88	70%	14.62	-0.24
KLX03	–922.45	964.5	975.15	12.57	19.24	70%	13.47	-0.90
KLX08	–320.03	396	400.87	4.56	7.19	10%	0.75	3.81
KLX08	–390.73	476	485.65	15.57	52.03	10%	5.40	10.17
KLX08	–504.54	609	618.51	17.57	72.47	10%	7.52	10.05
KLX13A	–408.01	432	439.16	7.38	51.01	32%	16.32	-8.94
KLX13A	–474.99	499.5	506.66	27.39	172.27	32%	55.13	-27.74
KLX15A	–467.22	623	634.51	12.9	19.79	58%	11.41	1.49
KLX17A	–342.32	416	437.51	22.12	24.09	67%	16.14	5.98

Depending on how much drill water was ingested and other hydraulic characteristics of the fracture, the composition will change gradually, or rapidly, to that of a groundwater mixed with drill water. From then on, further pumping should lower the concentration of tracer but the rate of lowering is not only dependent on the quantity that was injected but also on the extent of dilution by mixing. For instance, the injected water that has entered as an unbroken slug of water as it pushes the ambient groundwater ahead of it should, therefore, return as the same. Alternatively, the injected water may have immediately split into several pathways in the bedrock and mixed with ambient groundwater before returning. Furthermore, the injected water may been subject to local hydraulic gradients and migrated away from the borehole, only returning under high pumping and drawdown conditions.

6 Calculations using volumetric data

As shown in Table 5-1, the flushing water volumes entering the fractures during drilling can be calculated only for 5 sections: 3 sections in KLX08, one section in KLX15A and one section in KLX17A. For the other sections, the return water is higher than the drilling water, making the calculations impossible. The calculations below are based on the data from Tables 4-1 and 5-1 and the sampling events logs and volumes provided by Geosigma (Appendix 1).

KLX08

1) section 396–400.87
   The calculated volume left in the fracture is 3.81 m^3 with 87% concentration of the nominal drilling water. During sampling, 6.1 m^3 were pumped out, which is more than necessary in order to remove the drilling water. This is confirmed by the sample 10794 which has 0.86% of drilling water.
2) section 476–485.65
   The calculated volume left in the fracture is 10.17 m^3 with 93% concentration of the nominal drilling water. During sampling 4 m^3 were pumped out, and 20.2% of drilling water in sample 10732 was found. The pumping should have continued in order to remove the additional drilling water from the section. Instead, due to the large amount of flushing water, the investigation was interrupted. A clean-up pumping applied to the entire borehole was performed, removing 2,068 m^3. After a new attempt, a second clean-up was made to the lower half of the borehole, removing an additional 356 m^3. The sampling was then performed.

Sample 10959 has 5.17% drilling water. As the clean-up was applied to the entire borehole, it is not possible to calculate how much volume was pumped out from this section. Therefore the calculations can not be completed.

3) section 609–618.51
   The calculated volume left in this fracture is 10.05 m^3 with 99% concentration of the nominal drilling water. During sampling 4.3 m^3 were pumped out. The pumping should have continued in order to remove the additional drilling water from the section. Instead, due to the large amount of flushing water, the investigation was interrupted. A clean-up pumping applied to the entire borehole was performed, removing 2,068 m^3. After another attempt, a second clean-up was made to the lower half part of the borehole removing an additional 356 m^3. The sampling was then performed. Sample 11211 has 10.9% drilling water. As the clean-up was applied to the entire borehole, it is not possible to calculate how much volume was pumped out from this section. Therefore the calculations can not be completed.

KLX15A

1) section 632–634.51
   The calculated volume left in the fracture is 1.49 m^3 with 42% concentration of the nominal drilling water. During sampling, 4.47 m^3 were pumped out, more than the calculated volume which would have been necessary to pump out in order to remove the drilling water. The sample 11928, taken after pumping this volume, has 7.55% drilling water. This is perhaps due to dilution and mixing of the drilling water in the formation water.

KLX17A

2) section 416–437.51
   The calculated volume left in the fracture is 5.98 m^3 with 54% concentration of the nominal drilling water. During sampling 3.16 m^3 were pumped out, corresponding to the calculated volume which could have been necessary to pump out in order to remove the drilling water. This is confirmed by the sample 11765 which has 1.18% of drilling water.

7 Discussion

It is important to have a stable tracer concentration in the injected drill water. The typical uncertainty in uranine concentrations is less than 5% for a single analysis but over the course of a drilling campaign (several months), may drift to 25%. In the drilling of all Laxemar boreholes a constant uranine injection rate was maintained although the boreholes were left open during and after drilling.

To improve the understanding of the hydrogeological system, it would be worthwhile monitoring the uranine concentration in return water during flushing (i.e. when injection due to drilling has ended and before pumping for sampling begins). This would indicate how much dilution of drill water has occurred, how easily it can be removed and how extensively it has penetrated the fracture network.

The uranine data appear to show that there is no single correlation or trend in uranine with major ion concentration. In the examination of Forsmark data, similar conclusions were reached although further complexity was added by the multiple testing by hydrological research group and the frequent use of saline water as a drilling and flushing fluid. Saline drilling water induced less change in the groundwater chemistry simply because it is nearer the chemistry of the groundwater than are low-salinity surface waters. The results obtained in the Laxemar DIS analyses more clearly showed changes in concentrations because of the use of a less saline drilling fluid.

Many graphs of major ion concentrations (Na^+, Ca^{2+}, Cl^-) versus time showed fairly constant concentrations during pumping for sampling, irrespective of uranine concentration or trend during pumping. Relative stability might be expected if a saline groundwater is used as a drill water tracer rather than a fresh water (from rivers, lakes, etc). These fluids typically had the composition of Baltic seawater with some modifications in Ca, Mg and Cl. However, it is more difficult to obtain useful DIS results if the drill water composition is not well-removed from that of the formation water.

The Drilling Impact Study as applied to the Laxemar site has shown that calculation of the drill water volume lost in the fractures during drilling is not possible if there is a lack of data on borehole flushing volumes. In this study, these data only became available from Sicada and P-reports at a late stage and it has now been possible to determine how much water should be pumped out from the sections before sampling. This type of water balance greatly helps and guides the sampling for chemical composition.

Pumping for groundwater sampling, after drilling and flushing is complete, has not always shown a decline in uranine concentration, as might be expected. Of the 11 sections tested in this study, uranine levels decreased, remained constant, or increased as water was removed (Table 4-2). Again, there appears to be no relationship with depth of zone (plotted here as length along the borehole). It might be expected that the lower permeability sections, which are typically found at depth, would show clearer trends, but this is not the case.

The correlation of trends in uranine content of drill water with expected trends in ionic species has also not been clearly and reproducibly seen in this study. Instead, as found at the Forsmark site, the tendency has been for major ion (Na^+, Ca^{2+}, Cl^-) concentrations to remain constant or only slightly changing (sometimes in the wrong direction) as uranine content changes in response to pumping. Minor ions, however, (in particular, Mg^{2+} and SO_4^{2-}) were less prone to vary and this may be due to various extents of mixing with more dilute waters from the upper ~ 500 m.

It might be concluded from this study that the use of uranine as a drill water tracer and chemical indicator will not give consistent results. The following factors may impede the success of uranine as a drill water tracer:

1. Use of a drilling water that has a composition close to saline water at ~ 500 m depth.
2. Problems inherent in monitoring tracer injection and withdrawal.
3. The practice of leaving borehole sections open to each other between testing periods.
4. The possibility of non-conservative behaviour of uranine (interaction with clays, dissolved organics, etc).

The use of uranine as a groundwater tracer in saturated, fractured rock is questionable because of the results of the Forsmark and Laxemar studies described here. The expected trends in ion chemistry as a result of removing drill water by continued pumping are often not seen in the database and it is equally possible that ionic concentrations remain constant or even increase as the percentage of drill water is decreased.

Despite the above problems, the use of uranine as a conservative drill water tracer should be continued so that a more extensive database of its behaviour can be assembled. Monitoring of the often extensive period during flushing, after the end of drilling, is recommended in future work to fill in the data gap between drill stoppage and chemical sampling. Correlation of uranine trends with those seen in hydrochemical data may help to resolve some of these difficulties, especially if dilute drilling fluids can be used. It is clear though, that uranine concentration is not an ideal parameter on which to base acceptance or rejection of a suite of chemical analyses in groundwater, for use in calibrating hydrochemical and hydrogeological models. Stability of dissolved ion concentration is at least as important as a guide and this approach is used for determining representative groundwater samples (John Smellie, pers. comm.).

8 Conclusions

The Drilling Impact Study (DIS) has been developed and tested by the ChemNet group to further the understanding of the effects of drill water on ambient groundwater chemistry. Smellie and Tullborg (personal communication) have addressed this issue, in part, and their efforts have focused on preparing documents describing each borehole at the Forsmark and Laxemar sites in terms of geology, hydrogeology and hydrochemistry. They have summarised data available from Sicada to obtain a broad understanding of the impact of drill water on groundwater composition.

An in-depth study of selected borehole sections at the Forsmark site was performed by /Gascoyne and Gurban 2008/ in which mixing with drill water was described mathematically so that residual volumes of drill water in fractures in the host rock could be calculated and adjustments made to groundwater composition, if necessary.

DIS has shown that it is a useful tool to evaluate the response of drilling on groundwater composition and redox potential, provided that certain precautions are taken (e.g. use of a non-saline drill water, longer monitoring periods, etc). DIS has also shown that modelling of the data, particularly time-series data, and comparison with measured data, can be performed with some degree of success, but again relies on there being a long-term record of data, the use of fresh water as a drilling water (so that the effect of small volumes of diluting fluid can more easily be seen) and isolation of the test interval from surface effects and contaminations.

A detailed sensitivity analysis has not been conducted on the DIS performed so far because of the unforeseen problems realised during the course of analysis (e.g. introduction of unquantified contaminants or by other groups, imprecise knowledge of injection concentrations (a factor in the Forsmark study, mainly) and lack of flushing data in Sicada (for Laxemar). In the estimation of the authors, we believe that sampling and chemical analysis of groundwaters become worthless when the content of uranine exceeds about 25%.

The question of what to do about the high salt content of drill waters cannot be answered at this time because some of the Forsmark and Laxemar groundwaters were contaminated by hydrogeological activities, complete flushing data were only recently available for Laxemar, and hydrochemical time-series data often do not show any significant changes or trends despite significant reduction of drill water content during pumping.

It was noted in the in section 2 of this report that the DIS study for Laxemar should try to answer the anomalies and questions raised in this project. Responses to these questions and estimations as to whether DIS has succeeded are as follows:

1) **Response evaluation:** This task involves detailed evaluation of analyses of samples from repository depth in order to study the behaviour of major ionic components and redox sensitive elements. Work done on the Forsmark site has shown that drill water injection can be monitored with success during and after drilling but the observed trends are not always comparable with one another.
2) **Response modelling:** Time-series analysis has been performed for Forsmark and Laxemar boreholes with reasonable success by modelling the injection of drilling water and comparing the results with measured data. However, as noted in 1) above, modelling results do not always match those observed in the field and further work is needed to resolve the reasons for this.
3) **Sensitivity analyses:** In addition to analytical precision and accuracy of flow measurements, important questions must be addressed such as how much drilling water can be injected before the composition of deep groundwater becomes compromised. This is especially a problem if drilling water is itself brackish or saline. Evidence from Forsmark and Laxemar suggests that the results are highly dependent on the composition of the drill water and this needs to be carefully examined in all future work.

4) **Overall evaluation:** The overall utility of the DIS method can be evaluated if the following aspects can be satisfactorily addressed: Is the injection of drill water stable and well-monitored; Do trends in the chemical/isotopic/redox data agree with modelled results; Can samples with high drilling water content be used for modelling?

   In conclusion, DIS has an important place in site characterisation studies but the work described here has shown that simple, expected trends and correlations are often not found and, even, that the opposite relationships are clearly occurring.

The advices and support from Marcus Laaksoharju, John Smellie. Eva-Lena Tullborg and Bill Wallin are acknowledged.

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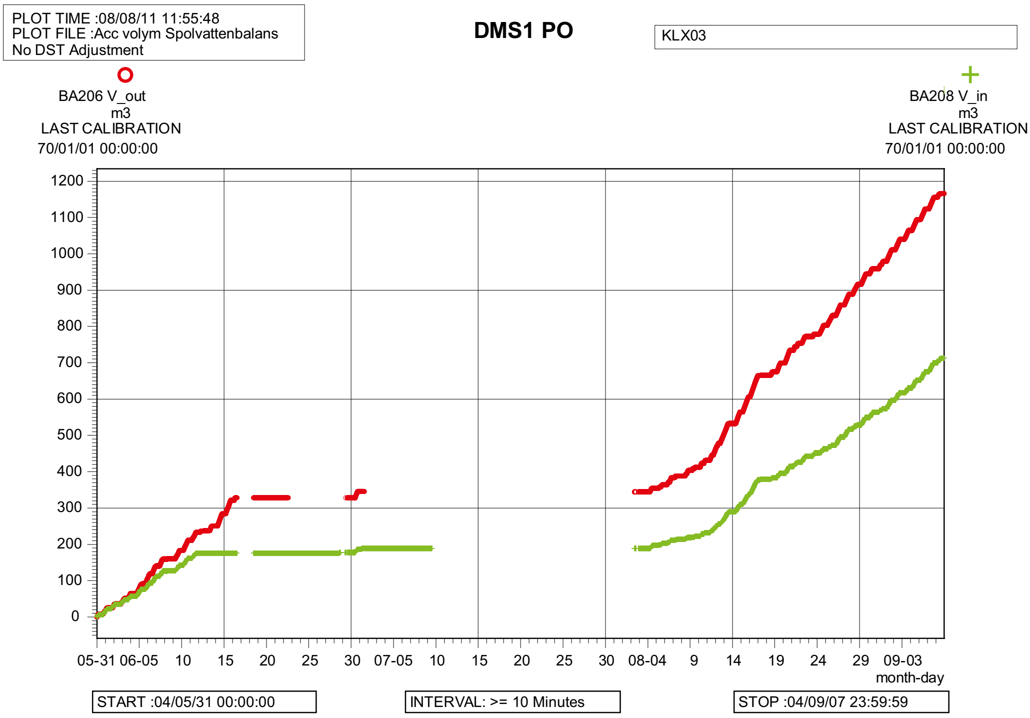
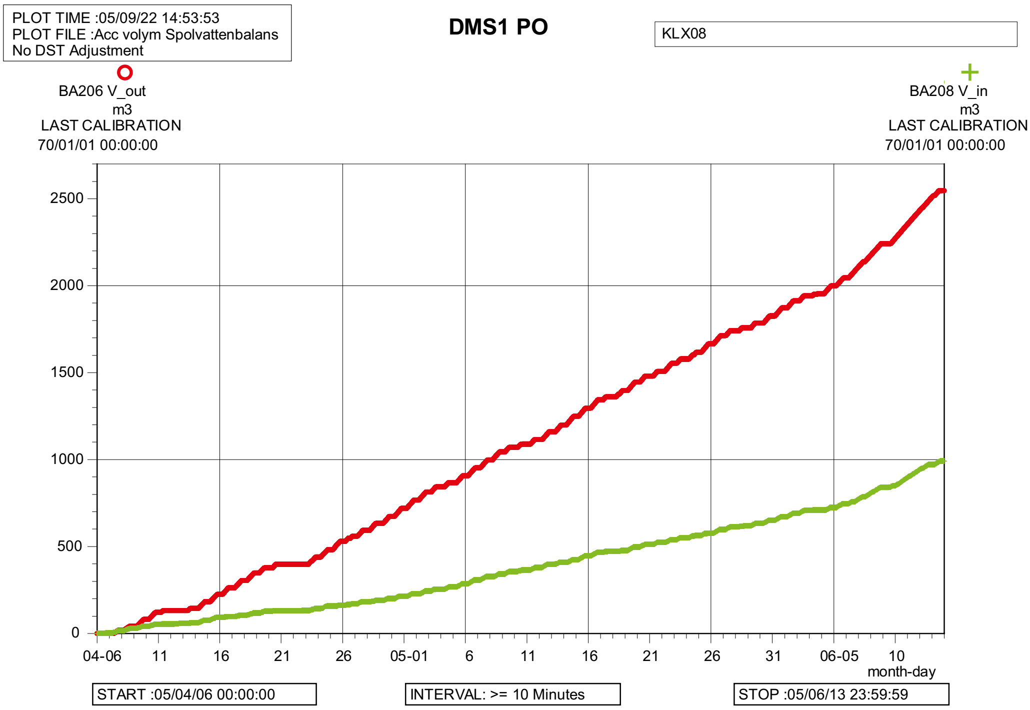
Appendix 1

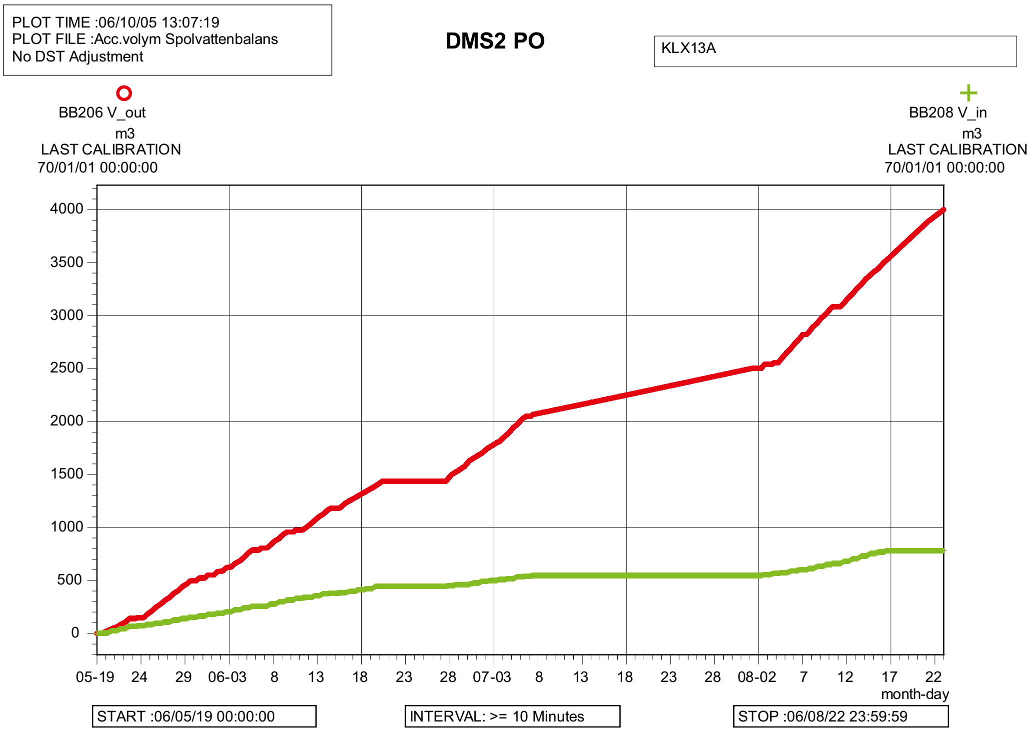
(1) Diagrams showing injected and withdrawn drill water for five Laxemar boreholes. The plots are obtained from Sicada and DMS databases. (2) Tables showing the Investigation sequence in KLX08 and KLX17A. The tables are obtained from Geosigma.



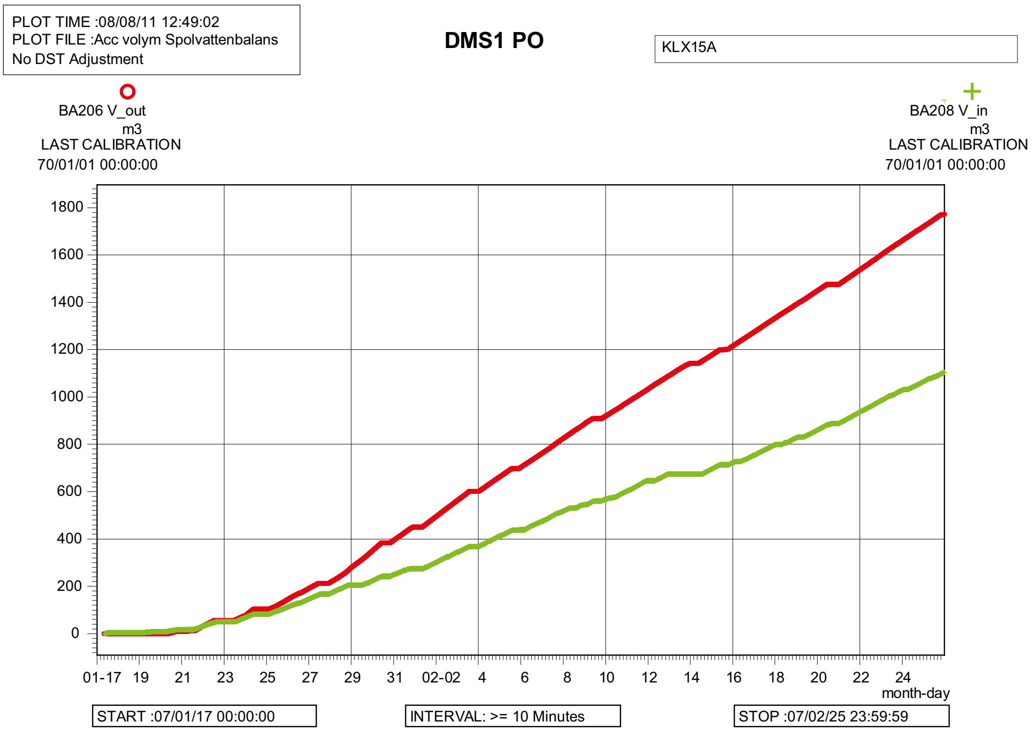
KLX03 Plot Accumulated volumes flushing and returned water.



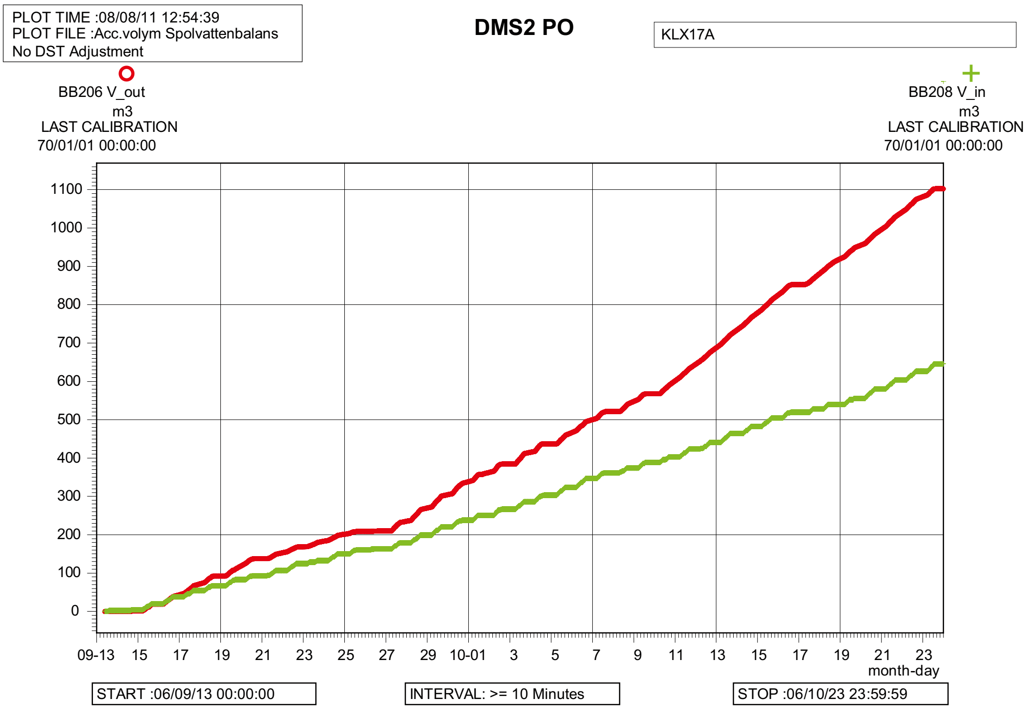
KLX08 Plot Accumulated volumes flushing and returned water.



KLX13A Plot Accumulated volumes flushing and returned water.



KLX15A Plot Accumulated volumes flushing and returned water.



KLX17A Plot Accumulated volumes flushing and returned water.

KLX08

Table A1. From Geosigma. Investigation sequence in KLX08.

Start date/ Stop date	Section (m)	Comment
2005-11-22/ 2006-12-20	197.00–206.65	Pumped volume = 6.3 m^3 Flow rate approx. 180 mL/min
2006-01-03/ 2006-01-17	476.00–485.65	Pumped volume = 4.0 m^3 Flow rate approx. 40–200 mL/min Interrupted investigation
2006-01-17/ 2006-02-01	610.00–619.65	Pumped volume = 4.3 m^3 Flow rate approx. 200 mL/min Interrupted investigation
2006-02-02/ 2006-03-07	396.00–400.87	Pumped volume = 6.1 m^3 Flow rate approx. 150–190 mL/min
2006-03-08/ 2006-03-28	0–1,000.41	Clean-up pumping Pumped volume = 2,068 m^3 Flow rate approx. 77–84 L/min
2006-03-30/ 2006-04-03	610.00–619.62	Interrupted investigation
2006-04-03/ 2006-04-25	476.00–485.62	Pumped volume = 5.8 m^3 Flow rate approx. 200–250 mL/min Interrupted investigation
2006-05-03/ 2006-05-09	599.27–1,000.41 473.37–1,000.41	Clean-up pumping
2006-05-09/ 2006-05-17		Pumped volume = 356 m^3 Flow rate approx. 1,523 L/min
2006-05-18/ 2006-06-27	476.00–485.62	Pumped volume = 7.7 m^3 Flow rate approx. 200 mL/min
2006-06-27/ 2006-07-27	609.00–618.51	Pumped volume = 5.2 m^3 Flow rate approx. 70–150 mL/min

Interrupted investigation in section 476.0–485.6 (1) m

Table A2. Events during the pumping/measurement period in section 476.0–485.6 (1) m.

Date	Event	Sample no.
060102	Calibration of borehole Chemmac	
060103	**Lowering of downhole equipment S2 (476.00–485.65 m)**	
060104	Calibration of surface Chemmac	
060105	Water sampling: SKB class 2; pH, electrical conductivity, alkalinity, chlorinity and Uranine	10730
060109	Water sampling: Uranine	10731
060110	Water sampling: SKB class 4	10732
060111	Water sampling: Uranine	10733
060112	Water sampling: SKB class 4	10734
060113	Driving pump exchanged, due to leakage of oil	
060116	Water sampling: Uranine	10735
060117	Oxygen meter; cleaning and exchange of membrane, calibration	
	Interrupted investigation due to large amounts of flushing water	
	End of Chemmac measurement	
060201	Calibration of borehole Chemmac	
060202	Calibration of surface Chemmac	

Interrupted investigation in section 610.0–619.6 (1) m

Table A3. Events during the pumping/measurement period in section 610.0–619.65 (1) m.

Date	Event	Sample no.
060102	Calibration of borehole Chemmac	
060104	Calibration of surface Chemmac	
060117	**Lowering of downhole equipment (610.00–619.65 m)**	
060118	Water sampling: Uranine	10736
060119	Water sampling: Uranine	10739
060123	Water sampling: Uranine	10737
060124	Water sampling: SKB class 2; pH, electric conductivity, alkalinity, chlorinity, anions and Uranine	10738
060127	Water sampling: SKB class 2; pH, electrical conductivity, alkalinity, chlorinity and Uranine	10740
	Interrupted investigation due to large amounts of flushing water	
050201	**End of Chemmac measurements**	
	Raising equipment	
	Calibration of borehole Chemmac	
060202	Calibration of surface Chemmac	

Table A4. Events during the pumping/measurement period in section 396.0–400.9 m.

Date	Event	Sample no.
060201	Calibration of borehole Chemmac	
060202	**Lowering of downhole equipment (396.00–400.87 m)**	
060202	Calibration of surface Chemmac	
	Start of Chemmac measurements	
060203	Water sampling: SKB class 2	10741
060207	Water sampling: SKB class 5	10794
060209	Water sampling: SKB class 4	10795
060210	Humic and fulvic acids; enrichment start	
060213	Low water flow from borehole pump (120 mL/min)	
060214	Water sampling: SKB class 5	10742
	Surface Chemmac temporary not in use due to exchange of electrode holder	
060217	Water sampling: SKB class 4	10743
060220	Water sampling: SKB class 5	10744
060220	Leakage of oil from the driving pump	
060221	Humic and fulvic acids; fractionation 1 kD	10746
060222	Humic and fulvic acids; fractionation 5 kD	10746
060223	Water sampling: SKB class 4	10745
060227	Water sampling: SKB class 5	10746
	A SKB class 5 control sample was not collected due to low water flow (35 mL/min)	
	PVP-sampler: opening of valve at 17:00	
060228	PVP-sampler: closure of valve at 06:40	
	Sampling for microbes and dissolved gases, however, the PVB containers were not sent for analysis due to small volumes of sampled water in two PVBs and low pressure in one PVB	
	Sampling for colloids, one PVB container. Only the results from the second sampling occasion with two PVB containers are reported	
	End of Chemmac measurements	
	Raising equipment	
	Calibration of borehole Chemmac	
	Prolonged measurement due to defective PVP equipment	
	Lowering of downhole equipment (369.00–400.87 m)	
060301	Calibration of surface Chemmac	
060306	Water sampling: SKB class 5, all options	10747
	Water sampling: SKB class 5, control sample	10748
	Humic and fulvic acids; enrichment stop	
	PVP-sampler: opening of valve at 17:30	
060307	PVP sampler: closure of valve at 06:11	
	Sampling for colloids, microbes and dissolved gases	10747
	End of Chemmac measurements	
	Raising equipment	
	Calibration of borehole Chemmac	
	Calibration of surface Chemmac	
060308-060328	Clean-up pumping (0–1,000.41 m) Water sampling: SKB class 1; Electrical conductivity and Uranine	10868, 10870, 10871, 10884, 10890, 10898, 10901, 10903, 10904, 10908, 10923, 10933, 10934, 10939

Interrupted investigation in section 610.0–619.6 (2) m

Table A5. Events during the pumping/measurement period in section 610.0–619.6 (2) m.

Date	Event
060329	Calibration of borehole Chemmac
060330	**Lowering of downhole equipment (610.00–619.62 m)**
060331	Calibration of surface Chemmac
060403	**End of chemmac measurements** **Raising equipment from 610.00–619.62 to 476.00–485.62 m**

Interrupted investigation in section 476.0–485.6 (2) m

Table A6. Events during the pumping/measurement period in section 476.0–485.6 (2) m.

Date	Event	Sample no.
060329	Calibration of borehole Chemmac	
060331	Calibration of surface Chemmac	
060403	**Raising equipment from 610.00–619.62 to 476.00–485.62 m**	
060404	Water sampling: SKB class 2; pH, electrical conductivity, alkalinity, chlorinity and Uranine	10750
060406	Water sampling: SKB class 4	10954
060408	Defective spring in borehole pump	
060413	Water sampling: SKB class 1; Uranine	10955
060412	**Raising equipment**	
	Exchanged borehole pump	
	Lowering of downhole equipment (476.00–485.62 m)	
060418	Water sampling: SKB class 4	10956
060420	Water sampling: SKB class 2; pH, electrical conductivity, alkalinity, chlorinity and Uranine	10957
060424	Water sampling: SKB class 2; pH, electrical conductivity, alkalinity, chlorinity and Uranine	10958
	Interrupted investigation due to large amounts of flushing water	
060425	**Raising of equipment**	
	Calibration of borehole Chemmac	
	Calibration of surface Chemmac	
060503-060517	Clean-up pumping (599.27–1,000.41 m and 473.37–1,000.41 m)	11015-26 and
	Water sampling: SKB class 1; Electrical conductivity and Uranine	11027-11028, 11045-11056

Table A7. Events during the pumping/measurement period in section 476.0–485.6 (3) m.

Date	Event	Sample no.
060518	Calibration of borehole Chemmac	
060519	**Lowering of downhole equipment S2 (476.00–485.62 m)**	
060522	Water sampling: SKB class 4	10959
	No connection with PVP equipment	
	Calibration of surface Chemmac	
060523	Calibration of oxygen meter	
060524	Water sampling: SKB class 4	11087
	Low water flow due to leakage of water in borehole pump	
060529	**Raising equipment**	
	Exchange of borehole pump and PVP	
	Lowering of downhole equipment S2 (476.00–485.62 m)	
060530	Water sampling: SKB class 5	11094
	No electric power supply due to thunderstorm	
060531	**Raising equipment**	
	Low water flow due to defect spring in borehole pump. Exchange of borehole pump	
	Lowering of downhole equipment S2 (476.00–485.62 m)	
060601	Water sampling: SKB class 4	11088
	Humic and fulvic acids; enrichment start	
060607	Water sampling: SKB class 5	11115
060609	Water sampling: SKB class 4	11118
060612	Water sampling: SKB class 5	11143
060612	Humic and fulvic acids; fractionation 1 kD	11183
060613	Humic and fulvic acids; fractionation 5 kD	11183
060615	Water sampling: SKB class 4	11158
060619	Water sampling: SKB class 5	11159
060621	Water sampling: SKB class 4	11178
060626	Water sampling: SKB class 5, all options	11183
	Water sampling: SKB class 5, control sample	11160
	Humic and fulvic acids; enrichment stop	
	PVP-sampler: opening of valve at 12:18	
060627	PVP-sampler: closure of valve at 06:37	
	Sampling for colloids, microbes and dissolved gases	11183
	End of Chemmac measurements	
	Raising equipment	
	Calibration of borehole Chemmac	
	Calibration of surface Chemmac	
061128	A 250 ml archive sample with SKB number 11087 (new SKB number 11540) are sent to University of Waterloo in Canada for re-analysis of ^{3}H	11540
061227	A 250 ml archive sample with SKB number 11087 (new SKB number 11548) are sent to a laboratory in Krakow, Poland, for analysis of ^{3}H	11548
070202	A 250 ml sample of deionised water from the tank for the driving water pump and hydraulic borehole pump is analysed for ^{3}H at Clab (laboratory at SKB)	11685
070207	A 250 ml sample of deionised water from the tank supplying the smaller tank for the driving water pump and hydraulic borehole pump is analysed for ^{3}H at Clab (laboratory at SKB)	11686

Table A8. Events during the pumping/measurement period in section 609.0–618.5 (3) m.

Date	Event	Sample no.
060627	**Calibration of borehole Chemmac**	
060628	**Lowering of downhole equipment S2 (609.00–618.51 m)**	
	Calibration of surface Chemmac, Addition of an oxygen electrode after the svivel in S2 for comparison with the oxygen electrode in MYC2 Manual readings	
060629	Water sampling: SKB class 2	11205
060630	Water sampling: Uranine	11207
060703	Water sampling: SKB class 4	11211
060706	Water sampling: SKB class 4	11216
	Loss of contact with borehole Chemmac	
060710	Water sampling: SKB class 4	11218
060712	**Raising equipment**	
	Re-calibration of oxygen electrode in MYC2	
	Disconnection and repair of borehole Chemmac	
	Lowering of downhole equipment S2 (609.00–618.51 m)	
060713	Low water flow caused by leakage in swivel, repair	
060714	Water sampling: SKB class 4	11219
060717	Water sampling: SKB class 5	11222
060720	Water sampling: SKB class 4	11229
060724	Water sampling: SKB class 5	11226
060725	Defrosting of cooling equipment in S2	
060726	Water sampling: SKB class 5, all options	11228
	Water sampling: SKB class 5, control sample	11227
060726	PVP-sampler: opening of valve at 15:25	
060727	PVP-sampler: closure of valve at 06:06	
	Sampling for colloids and dissolved gases	11228
	End of Chemmac measurements	
	Raising equipment	
	Calibration of surface Chemmac	

KLX17A

Table A9. From Geosigma. Events during the pumping/measurement period in section 416.0–437.5 m.

Date	Event	Sample no.
070301	Calibration of borehole Chemmac and surface Chemmac. Exchange of oxygen electrode	
070302	**Lowering of downhole equipment S2 (416.00–437.51 m)**	
	Start of borehole pump and Chemmac measurements	
070305	Water sampling: Uranine	11763
070306	Water sampling: SKB class 2	11764
070308	Alarm regarding low water flow	
070309	**Lifting**	
	Replacement of broken spring in the borehole pump.	
	Lowering of downhole equipment S2 (416.00–437.51 m)	
	Start of borehole pump and Chemmac measurements	
070312	Water sampling: SKB class 5 The sample for U and Th is stored in the archive	11765
	The current to the borehole Chemmac is switched off due to high current consumption. Restart of the measurement application	

Date	Event	Sample no.
070313	Humic and fulvic acids; enrichment start	
070315	Water sampling: SKB class 4	11766
070319	Water sampling: SKB class 5 The sample for U and Th is stored in the archive	11767
070320	Humic and fulvic acids; fractionation 1,000 D	11810
	Change of conductivity scale from 2,000 mS/m to 500 mS/m.	
070321	Water sampling: SKB class 5 The sample for U and Th is stored in the archive	11768
	Humic and fulvic acids; fractionation 5,000 D	11810
070323	Water sampling: SKB class 4	11769
070326	**Lifting**	
	Alarm regarding low water flow. Replacement of broken spring in the borehole pump	
	Lowering of downhole equipment S2 (416.00–437.51 m)	
	Start of borehole pump and Chemmac measurements	
070327	**Lifting**	
	Leakage of water from the packers. Repair	
	Calibration of borehole Chemmac	
	Lowering of downhole equipment S2 (416.00–437.51 m)	
	Start of borehole pump and Chemmac measurements	
070328	Calibration of surface Chemmac	
070330	Water sampling: SKB class 4	11770
070402	Water sampling: SKB class 5 The sample for U and Th is stored in the archive	11771
070404	Water sampling: SKB class 4	11772
070410	Low water flow due to defective driving pump. Repair. Change of relay.	
070411	Water sampling: SKB class 1; pH, conductivity, alkalinity, chlorinity, Uranine, Cl^-, Br^-, F^- and SO_4^{2-}	11773
070412	Water sampling: SKB class 5 The sample for U and Th is stored in the archive	11809
070416	**Lifting**	
	Alarm regarding low water flow. Replacement of broken spring in the borehole pump	
	Lowering of downhole equipment S2 (416.00–437.51 m)	
	Start of borehole pump and Chemmac measurements	
070418	Water sampling: SKB class 5; all options	11810
	Water sampling: SKB class 5, control sample. Density measurement	11811
	PVP-sampler: opening of valve at 17:24	
070419	PVP-sampler: closure of valve at 06:36	
	Residual current operated circuit breaker	
	Humic and fulvic acids; enrichment stop	11810
	Lifting	
	Sampling for microbes and dissolved gases	11810
	Lowering of downhole equipment S2 (416.00–437.51 m)	
	Start of borehole pump and Chemmac measurements	
070423	Water sampling: SKB class 5 The sample for U and Th is stored in the archive	11812
	PVP-sampler: opening of valve at 14:22	
070424	PVP-sampler: closure of valve at 06:35	
	Sampling for colloids	11810
	End of Chemmac measurements	
	Lifting	
	Calibration of borehole Chemmac and surface Chemmac	

Appendix 2

Table of groundwater chemical compositions in 10 sections of Laxemar borehole.

Section Number	ID CODE	SAMPLE DATE	ELEVATION (MID)	COMMENTS	CLASS NO	Drilling water residue (%)	pH (lab)	Electric Conductivity (mS/m)	SEC UP (m)	SEC LOW (m)	Relative charge balance (%) from SICADA	Na	K	Ca
1	KLX03	02/21/05	–379.85	Cat 3, possible instability, borehole used later for tracer	4	3.30	7.99	380.0	408.00	415.30	1.95	631	5.2	167
	KLX03	02/24/05	–379.85		5	2.84	7.94	448.0	408.00	415.30	1.42	732	5.9	214
	KLX03	02/28/05	–379.85		4	2.31	7.98	469.0	408.00	415.30	1.09	759	5.8	225
	KLX03	03/11/05	–379.85		4	1.71	7.86	446.0	408.00	415.30	0.97	719	5.7	209
	KLX03	03/14/05	–379.85		4	2.06	7.79	487.0	408.00	415.30	1.07	780	5.8	232
	KLX03	03/17/05	–379.85		4	1.95	7.89	492.0	408.00	415.30	1.57	797	5.5	241
	KLX03 (R)	03/22/05	–379.85		5	1.88	7.89	469.0	408.00	415.30	2.12	791	5.5	234
2	KLX03	04/01/05	–700.60	Cat 5, unstable, possible short cutting, borehole used later for tracer ts tests	4	6.83	7.49	731.0	735.50	748.04	1.17	969	9.8	579
	KLX03	04/04/05	–700.60		4	8.66	7.50	982.0	735.50	748.04	–2.17	1,130	9.8	861
	KLX03	04/07/05	–700.60		4	9.67	7.49	1,060.0	735.50	748.04	0.01	1,300	11.4	974
	KLX03	04/15/05	–700.60		5	10.20	7.38	909.0	735.50	748.04	–1.60	1,130	10.9	784
	KLX03	04/18/05	–700.60		4	10.20	7.35	1,090.0	735.50	748.04	0.09	1,320	11.6	1,050
	KLX03	04/21/05	–700.60		5	10.60	7.39	1,130.0	735.50	748.04	–2.49	1,380	11.1	993
	KLX03	04/25/05	–700.60		5	10.80	7.41	1,200.0	735.50	748.04	–0.63	1,450	10.9	1,090
3	KLX03	01/24/05	–922.45	Cat 1, should be very good, borehole used later for tracer tests	2	0.15	8.64	2,760.0	964.50	975.15				
	KLX03	01/25/05	–922.45		4	0.13	8.65	2,790.0	964.50	975.15	1.32	2,860	8.5	3,800
	KLX03	01/27/05	–922.45		5	0.12	8.65	2,800.0	964.50	975.15	0.86	2,860	8.6	3,730
	KLX03	02/04/05	–922.45		5	0.06	8.66	2,810.0	964.50	975.15	0.74	2,850	8.7	3,730
	KLX03	02/07/05	–922.45		4	0.05	8.68	2,790.0	964.50	975.15	0.94	2,860	8.5	3,750
	KLX03	02/10/05	–922.45		5	0.07	8.65	2,790.0	964.50	975.15	–13.89	2,090	5.9	2,800
	KLX03 (R)	02/14/05	–922.45		5	0.04	8.68	2,800.0	964.50	975.15	0.89	2,880	8.6	3,780
	KLX03	02/14/05	–922.45		5	0.04	8.68	2,780.0	964.50	975.15				
4	KLX08	02/07/06	–320.03	Cat 5 short circuiting between section hosting young meteoric recharge groundwater	5	0.86	8.22	55.0	396.00	400.87	–0.15	99	2.8	18
	KLX08	02/09/06	–320.03		4	0.95	8.25	55.2	396.00	400.87	–0.76	100	2.8	18
	KLX08	02/14/06	–320.03		5	1.19	8.31	55.7	396.00	400.87	–0.82	102	2.6	17
	KLX08	02/17/06	–320.03		4	1.15	8.32	52.9	396.00	400.87	–1.28	102	2.5	16
	KLX08	02/20/06	–320.03		5	1.30	8.28	51.9	396.00	400.87	–0.70	103	2.5	15
	KLX08	02/23/06	–320.03		4	1.26	8.27	54.6	396.00	400.87	–1.12	102	2.4	16
	KLX08	02/27/06	–320.03		5	1.31	8.30	47.6	396.00	400.87	–1.93	101	2.6	16
	KLX08	03/06/06	–320.03		5	1.15	8.32	53.1	396.00	400.87	–1.01	103	2.4	15

Section Number	Mg	HCO3	Cl	SO4	Br	Fe	Fe TOT	Fe2+	Sr	H–2 (‰)	Tritium (TU)	O–18 (‰)	C–14 (pmc)	S–34 (‰)
1	8.9	223.00	1,040.0	96.80		0.8760	1.000	0.971	3.400	–97.2	–0.80	–12.50		
	10.4	204.00	1,290.0	116.00		1.0300	1.130	1.110	4.440	–96.5	–0.80	–12.80		15.7
	10.6	196.00	1,360.0	122.00		0.3550	0.385	0.371	4.690	–97.8	–0.80	–12.90		
	10.1	194.00	1,280.0	116.00		0.8140	0.816	0.816	4.280	–97.1	–0.80	–12.90		
	10.8	178.00	1,410.0	126.00		0.7790	0.783	0.791	4.780	–97.8	–0.80	–13.20		
	11.0	185.00	1,430.0	129.00		0.6820	0.732	0.717	4.920	–98.7	0.80	–13.30		14.7
	10.8	189.00	1,390.0	127.00		0.4080	0.435	0.429	4.840	–98.1		–13.00	65.20	15.1
2	11.2	113.00	2,250.0	232.00		1.7100	1.850	1.900	10.800	–100.1	–0.80	–12.60		
	11.8	65.50	3,180.0	311.00		0.8390	1.150	1.150	16.800	–100.4		–13.00		
	12.6	52.40	3,480.0	337.00		0.8960	1.040	1.030	18.900	–101.5	1.30	–13.20		
	12.9	76.40	3,010.0	305.00		1.8000	2.140	2.150	15.000	–100.0	1.00	–12.90		11.2
	13.2	45.10	3,630.0	373.00		1.1200	1.260	1.250	19.600	–102.1	–0.80	–13.20		
	12.9	38.00	3,820.0	391.00		1.0900	1.140	1.130	22.000	–91.7	0.90	–13.60	48.23	11.8
	12.8	33.50	3,940.0	398.00		0.8720	0.917	0.903	23.100	–92.1	1.20	–13.60	47.36	11.0
3		7.35	10,600.0											
	2.1	7.73	10,400.0	742.00		–0.1000	0.077	0.068	71.200	–93.4		–12.20		
	2.1	7.48	10,400.0	741.00		–0.0040	–0.005	–0.005	71.900	–94.8	–0.80	–12.20		12.4
	2.1	7.73	10,400.0	751.00		–0.0040	–0.005	–0.005	71.200	–94.9	–0.80	–12.20		11.3
	2.1	7.39	10,400.0	752.00		–0.1000	–0.005	–0.005	71.500	–94.0	–0.80	–12.20		
	1.6	7.74	10,500.0	749.00		–0.1000	–0.005	–0.005	52.000	–93.6	–0.80	–12.10		10.5
	2.1	7.70	10,500.0	758.00		–0.0040	–0.005	–0.005	72.200	–94.8	–0.80	–12.20		11.1
		7.95	10,400.0	749.00	109.000		0.013	–0.005						
4	3.2	287.00	14.3	13.80	–0.200	0.1480	0.129	0.124	0.286	–76.4	13.80	–10.70	66.04	33.7
	3.0	289.00	14.6	14.10	–0.200	0.1460	0.129	0.125	0.281	–76.2	5.40	–10.80	–	–
	2.7	291.00	14.9	14.60	–0.200	0.3720	0.359	0.351	0.273	–76.0	5.60	–10.70	65.64	33.9
	2.4	290.00	15.1	14.90	–0.200	0.6000	0.584	0.567	0.266	–77.2	6.10	–10.70	–	–
	2.4	287.00	15.2	15.00	–0.200	0.3620	0.346	0.328	0.262	–76.7	3.40	–10.80	65.57	31.1
	2.4	286.00	15.4	15.10	–0.200	0.0551	0.048	0.046	0.256	–76.8	4.30	–10.70	–	–
	2.5	287.00	15.6	15.20	–0.200	0.0266	0.034	0.023	0.258	–76.1	4.10	–10.70	63.69	29.1
	2.3	290.00	14.9	14.00	–0.200	1.0300	1.020	1.020	0.261	–76.4	5.40	–10.70	66.27	32.7

Section Number	ID CODE	SAMPLE DATE	ELEVATION (MID)	COMMENTS	CLASS NO	Drilling water residue (%)	pH (lab)	Electric Conductivity (mS/m)	SEC UP (m)	SEC LOW (m)	Relative charge balance (%) from SICADA	Na	K	Ca
5	KLX08	01/10/06	–390.73	Cat 2 Should be OK	4	20.20	7.88	346.0	476.00	485.65	0.78	524	5.1	176
	KLX08	01/12/06	–390.73		4	20.80	7.85	378.0	476.00	485.65	1.10	569	5.0	203
	KLX08	05/22/06	–390.71		4	5.17	7.84	498.0	476.00	485.62	–0.08	740	3.1	279
	KLX08	05/24/06	–390.71		4	4.93	7.89	488.0	476.00	485.62	–0.38	717	3.1	265
	KLX08	05/30/06	–390.71		5	5.33	7.51	493.0	476.00	485.62	0.71	764	3.2	286
	KLX08	06/01/06	–390.71		4	4.96	7.48	504.0	476.00	485.62	0.36	746	3.6	289
	KLX08	06/07/06	–390.71		5	5.33	7.75	512.0	476.00	485.62	–0.75	731	3.0	282
	KLX08	06/09/06	–390.71		3	5.39	7.83	513.0	476.00	485.62	–1.20	732	3.1	276
	KLX08	06/12/06	–390.71		5	5.38	7.83	512.0	476.00	485.62	–1.06	730	3.1	285
	KLX08	06/15/06	–390.71		4	5.44	7.80	517.0	476.00	485.62	1.16	789	3.7	282
	KLX08 (R)	06/19/06	–390.71		5	5.71	7.85	520.0	476.00	485.62	1.55	796	3.5	298
	KLX08	06/21/06	–390.71		4	5.82	7.85	520.0	476.00	485.62	0.00	769	3.7	282
	KLX08	06/26/06	–390.71		5	5.89	7.87	513.0	476.00	485.62	1.35	799	3.9	294
	KLX08	06/26/06	–390.71		5	5.98	7.84	516.0	476.00	485.62	–11.88	620	3.0	210
6	KLX08	07/03/06	–504.54	Cat 3 possible short-circuiting	3	10.90	8.10	636.0	609.00	618.51	0.79	955	6.0	381
	KLX08	07/06/06	–504.54		4	10.90	8.10	638.0	609.00	618.51	1.50	976	5.9	380
	KLX08	07/10/06	–504.54		4	10.90	8.15	650.0	609.00	618.51	1.04	966	5.8	378
	KLX08	07/14/06	–504.54		4	11.20	8.15	646.0	609.00	618.51	–1.02	929	5.7	364
	KLX08	07/17/06	–504.54		5	11.10	8.17	642.0	609.00	618.51	0.38	961	5.9	371
	KLX08	07/20/06	–504.54		4	11.20	8.18	643.0	609.00	618.51	0.11	960	6.2	365
	KLX08	07/24/06	–504.54		5	10.80	8.16	642.0	609.00	618.51	–0.47	949	6.4	360
	KLX08	07/26/06	–504.54		5	10.70	8.19	640.0	609.00	618.51	–0.46	947	5.9	367
7	KLX13A	12/18/06	–408.01	Cat 3 possible instability	4	11.30	8.24	263.0	432.00	439.16	–0.86	464	1.9	55
	KLX13A	12/21/06	–408.01		4	11.40	8.33	263.0	432.00	439.16	3.02	501	1.9	60
	KLX13A	01/04/07	–408.01		5	11.00	8.32	258.0	432.00	439.16	0.13	467	2.0	54
	KLX13A	01/08/07	–408.01		5	10.40	8.39	258.0	432.00	439.16	–0.79	458	1.8	52
	KLX13A	01/11/07	–408.01		5	10.20	8.35	259.0	432.00	439.16	–1.68	449	1.8	52
	KLX13A	01/17/07	–408.01		5	10.40	8.33	255.0	432.00	439.16	–0.85	449	1.8	51
	KLX13A	01/21/07	–408.01		5	8.75	8.41	257.0	432.00	439.16	0.33	463	1.8	52
8	KLX13A	11/23/06	–474.99	Cat 4 possible short-circuiting	4	14.10	7.82	242.0	499.50	506.66	–0.07	413	2.7	66
	KLX13A	11/28/06	–474.99		4	16.60	8.04	268.0	499.50	506.66	–0.47	469	2.3	66
	KLX13A	11/30/06	–474.99		4	16.10	8.07	268.0	499.50	506.66	–1.55	458	2.2	64

Section Number	Mg	HCO3	Cl	SO4	Br	Fe	Fe TOT	Fe2+	Sr	H–2 (‰)	Tritium (TU)	O–18 (‰)	C–14 (pmc)	S–34 (‰)	Sr–87/ Sr–86
5	8.2	95.10	1,000.0	92.40	4.760	0.5990	0.563	0.554	2.980	–98.2	1.70	–13.60	–	–	–
	8.3	82.20	1,110.0	97.60	5.280	0.5440	0.519	0.512	3.440	–102.7	1.90	–14.00	–	–	–
	6.9	34.80	1,530.0	132.00	7.600	0.6360	–	0.688	5.190	–115.1	95.20	–15.40	–	–	–
	6.6	34.00	1,480.0	128.00	7.400	0.3090	0.258	0.232	4.950	–111.9	756.60	–14.90	–	–	–
	7.2	34.10	1,550.0	133.00	7.950	0.6050	0.670	0.627	5.460	–115.2	2.90	–15.60	32.09	15.5	0.71572
	7.2	33.20	1,540.0	132.00	7.880	0.8530	0.810	0.794	5.230	–115.2	2.20	–15.60	–	–	–
	6.9	32.40	1,540.0	129.00	7.600	0.2440	0.244	0.213	5.110	–117.4	111.40	–15.40	–	15.6	0.71567
	6.7	33.50	1,550.0	131.00	7.670	0.2450	0.251	0.235	5.160	–117.1	52.30	–15.50	–	–	–
	6.7	32.20	1,560.0	130.00	7.630	0.2650	0.272	0.257	5.180	–114.0	38.90	–15.50	–	15.4	0.71568
	6.8	32.00	1,570.0	131.00	7.980	0.2250	0.280	0.237	5.410	–115.1	2.20	–15.70	–	–	–
	6.8	32.00	1,590.0	133.00	7.880	0.2980	0.295	0.288	5.510	–117.0	2.10	–15.60	–	17.0	0.71566
	6.8	32.70	1,580.0	131.00	7.870	0.2900	0.281	0.276	5.420	–116.1	2.00	–15.60	–	–	–
	6.9	32.30	1,600.0	132.00	7.980	0.2880	0.284	0.275	5.450	–116.1	2.10	–15.70	–	16.4	0.71567
	5.8	32.30	1,590.0	130.00	7.650	0.2200	0.284	0.278	4.600	–	–	–	–	–	–
6	8.4	20.20	2,010.0	141.00	9.850	0.0870	0.087	0.080	6.830	–115.4	1.60	–15.40	–	–	–
	9.1	20.10	2,010.0	138.00	9.550	0.0793	0.080	0.070	6.880	–115.1	–0.80	–15.40	–	–	–
	8.9	20.30	2,010.0	138.00	9.550	0.0360	0.039	0.032	6.770	–113.1	–0.80	–15.40	–	–	–
	8.7	20.20	2,020.0	144.00	10.700	0.1230	0.125	0.113	6.890	–114.2	2.30	–15.30	–	–	–
	9.0	20.10	2,020.0	144.00	10.300	0.2510	0.241	0.235	7.110	–114.4	1.70	–15.30	–	13.3	0.71555
	8.1	20.60	2,020.0	144.00	10.100	0.1310	0.127	0.125	6.940	–113.6	2.70	–15.30	–	–	–
	8.0	20.60	2,020.0	145.00	10.400	0.0062	–0.005	–0.005	6.850	–112.7	2.40	–15.30	–	13.2	0.71557
	8.0	20.50	2,030.0	145.00	10.600	0.0202	–0.005	–0.005	6.750	–112.9	2.50	–15.20	–	13.2	0.71556
7	3.4	70.50	762.0	37.30	3.880	0.0017	0.006	–0.006	1.210	–119.9	–0.80	–15.70			
	3.5	71.80	759.0	37.90	3.780	0.0017	–0.006	–0.006	1.280	–119.5	3.20	–15.80			
	3.2	74.10	745.0	36.50	3.430	0.0061	0.011	–0.006	1.210	–120.3	4.00	–15.70	29.07	28.6	0.71523
	3.1	73.70	744.0	36.50	3.520	0.0022	–0.006	–0.006	1.150	–119.3	3.10	–15.80	47.41	28.6	0.71522
	3.1	73.90	744.0	36.80	3.480	0.0024	–0.006	–0.006	1.160	–119.6	3.60	–15.90	21.71	29.0	0.71520
	3.0	75.30	728.0	37.10	3.650	0.0022	0.006	–0.006	1.130	–119.4	3.50	–15.80	23.69	28.5	0.71523
	3.2	74.60	733.0	35.90	3.600	0.3830	0.324	0.089	1.180	–118.7	11.50	–15.80	35.60	29.1	0.71524
8	5.5	97.70	678.0	43.30	3.550	1.5200	1.430	1.410	1.240	–107.1	10.20	–14.60			
	4.7	81.80	774.0	47.10	4.350	0.2190	0.212	0.198	1.340	–116.4	0.90	–15.10			
	4.4	83.70	769.0	47.30	4.220	0.2230	0.223	0.216	1.310	–114.0	1.90	–15.10			
	4.0	87.20	740.0	46.20	4.030	0.0303	0.045	0.044	1.230	–112.7	3.10	–15.20			

Section Number	ID CODE	SAMPLE DATE	ELEVATION (MID)	COMMENTS	CLASS NO	Drilling water residue (%)	pH (lab)	Electric Conductivity (mS/m)	SEC UP (m)	SEC LOW (m)	Relative charge balance (%) from SICADA	Na	K	Ca
9	KLX15A	06/28/07	–467.22	Cat 2 Should be OK	5	7.55	7.53	1,620.0	623.00	634.51	–0.78	2,090	13.5	1,430
	KLX15A	07/02/07	–467.22		5	6.66	7.48	1,660.0	623.00	634.51	–6.63	1,780	13.4	1,350
	KLX15A	07/04/07	–467.22		5	6.40	7.48	1,660.0	623.00	634.51	–0.33	2,110	13.4	1,460
	KLX15A	07/06/07	–467.22		4	6.46	7.04	1,660.0	623.00	634.51	–2.55	2,010	12.5	1,410
	KLX15A	07/09/07	–467.22		5	5.92	7.45	1,660.0	623.00	634.51	–1.98	2,050	12.7	1,440
	KLX15A	07/11/07	–467.22		4	5.75	7.53	1,660.0	623.00	634.51	0.01	2,070	13.2	1,560
	KLX15A	07/13/07	–467.22		4	5.58	7.22	1,670.0	623.00	634.51	–0.44	2,110	13.6	1,550
	KLX15A	07/16/07	–467.22		4	5.99			623.00	634.51		2,090	13.8	1,540
	KLX15A	08/01/07	–467.22		5	4.71	7.51	1,680.0	623.00	634.51	–1.43	2,060	13.0	1,550
	KLX15A	08/06/07	–467.22		5	4.43	7.42	1,690.0	623.00	634.51	–1.05	2,080	13.8	1,540
10	KLX17A	03/12/07	–342.32	Cat 3, possible instability	5	1.18	7.78	119.0	416.00	437.51	1.57	195	2.8	37
	KLX17A	03/15/07	–342.32		4	1.51	8.06	149.0	416.00	437.51	0.59	240	3.3	50
	KLX17A	03/19/07	–342.32		5	1.65	8.07	169.0	416.00	437.51	–2.56	265	3.5	54
	KLX17A	03/21/07	–342.32		5	1.67	8.11	269.0	416.00	437.51	–2.28	276	3.8	58
	KLX17A	03/23/07	–342.32		4	1.75	8.07	183.0	416.00	437.51	–3.71	273	3.6	57
	KLX17A	03/30/07	–342.32		4	0.98	7.72	120.0	416.00	437.51	2.11	195	2.9	40
	KLX17A	04/02/07	–342.32		5	1.60	7.85	174.0	416.00	437.51	–0.26	275	3.6	59
	KLX17A	04/04/07	–342.32		4	1.71	7.92	189.0	416.00	437.51	–1.84	292	3.7	61
	KLX17A	04/12/07	–342.32		5	1.80	7.96	217.0	416.00	437.51	–0.93	322	4.0	68
	KLX17A	04/18/07	–342.32		5	1.71	7.92	209.0	416.00	437.51	–0.78	329	4.0	68
	KLX17A	04/23/07	–342.32		5	1.72	7.95	214.0	416.00	437.51	–1.17	332	4.0	69

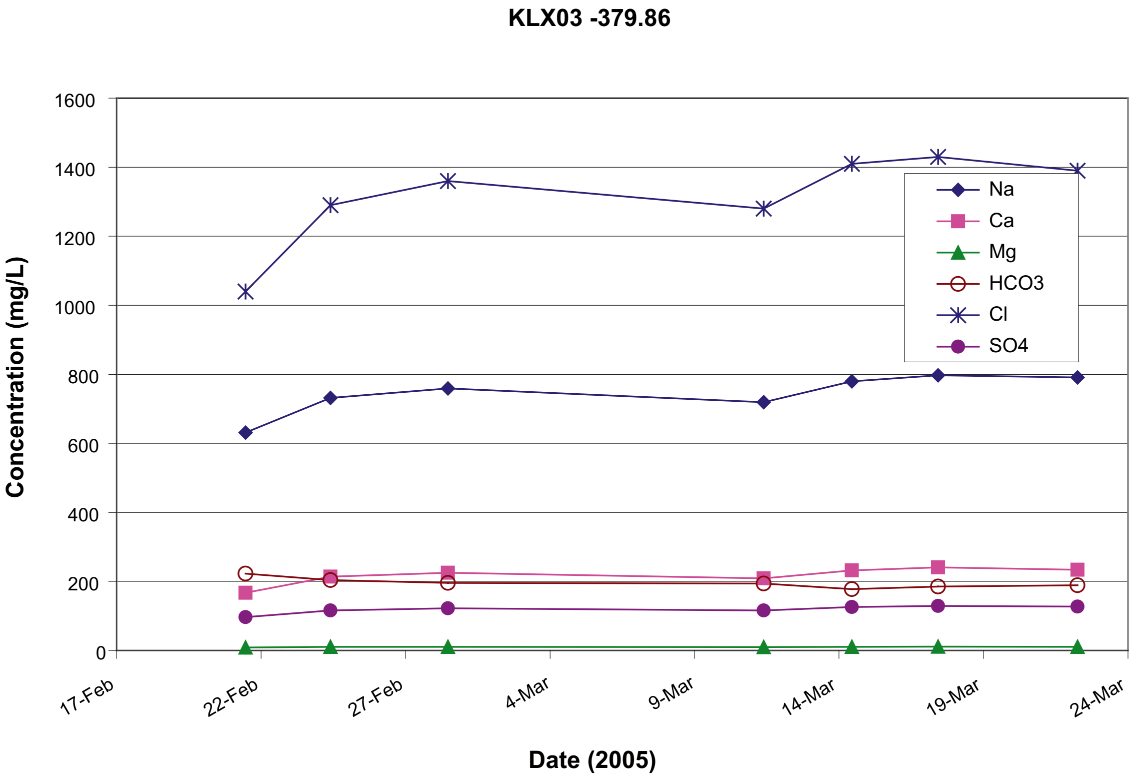
Section Number	Mg	HCO3	Cl	SO4	Br	Fe	Fe TOT	Fe2+	Sr	H–2 (‰)	Tritium (TU)	O–18 (‰)	C–14 (pmc)	S–34 (‰)	Sr–87/ Sr–86
9	52.8	17.00	5,670.0	408.00	29.900	0.7210	0.772	0.729	27.100	–79.9	1.00	–10.90		16.7	0.71562
	52.6	16.70	5,720.0	414.00	29.300	0.6150	0.596	0.631	26.600	–80.0	–0.80	–10.90		17.0	0.71562
	53.2	16.60	5,700.0	400.00	29.300	0.6500	0.690	0.676	27.500	–79.5	1.35	–10.90		16.7	0.71559
	50.7	15.60	5,740.0	417.00	31.100	0.5300	0.567	0.537	25.400	–79.0	–0.80	–10.90			
	52.0	16.00	5,790.0	430.00	28.800	0.6870	0.732	0.761	26.000	–79.3	1.08	–10.80		19.0	0.71559
	56.4	15.70	5,790.0	423.00	29.100	0.6790	0.725	0.696	26.900	–79.7	1.06	–10.70			
	55.8	16.00	5,890.0	415.00	28.600	0.2880	0.314	0.297	26.800	–79.5	1.23	–10.70			
	56.0		5,720.0	408.00	28.200	0.4660			26.400	–79.3	1.39	–10.70			
	53.9	14.80	5,920.0	407.00	28.000	0.4540	0.472	0.429	27.300	–79.8	0.92	–10.70		18.0	0.71560
	54.0	14.10	5,890.0	425.00	29.000	0.5370	0.556	0.548	27.700	–80.8	–0.80	–10.80		17.3	0.71561
10	6.0	183.00	254.0	13.70	0.980	2.3600	2.370	2.340	0.792	–93.6	6.24	–12.50	50.40	28.4	0.71527
	7.8	169.00	362.0	17.00	1.150	1.5400	1.480	1.450	1.110	–100.1	2.98	–13.10			
	8.3	154.00	450.0	19.10	1.560	1.0900	1.060	1.060	1.300	–102.8	2.44	–13.70	45.00	30.2	0.71525
	8.5	147.00	476.0	20.00	1.730	0.9740	0.987	0.956	1.400	–104.5	2.76	–13.90	44.20	30.3	0.71524
	8.4	142.00	490.0	20.60	1.770	0.8440	0.907	0.876	1.370	–105.6	2.56	–14.00			
	6.0	165.00	262.0	13.30	0.920	1.7400	1.700	1.700	0.846	–92.4	4.32	–12.30			
	8.3	140.00	455.0	19.40	1.640	1.3100	1.210	1.260	1.400	–103.2	4.58	–13.60	52.90	30.4	0.71524
	8.8	136.00	508.0	20.80	1.790	1.1100	0.980	1.050	1.490	–107.9	1.50	–14.30			
	9.4	122.00	565.0	22.90	2.000	0.7910	0.729	0.690	1.690	–111.1	0.90	–14.40	44.30	31.3	0.71522
	9.6	118.00	576.0	24.00	2.190	0.8760	0.892		1.690	–110.8	1.60	–14.40	42.60	32.1	0.71526
	9.8	115.00	591.0	24.40	2.250	0.8710	0.761	0.759	1.720	–110.9	1.30	–14.50	41.00	31.8	0.71519

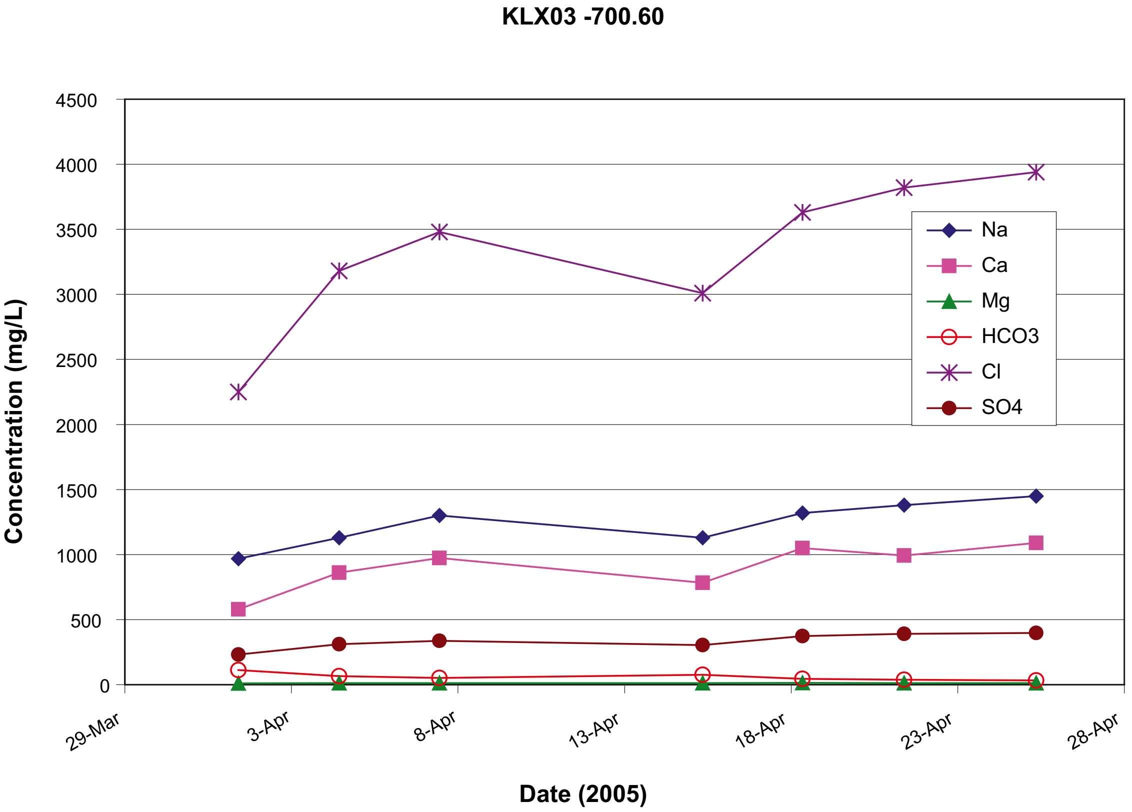
Drill water chemistry

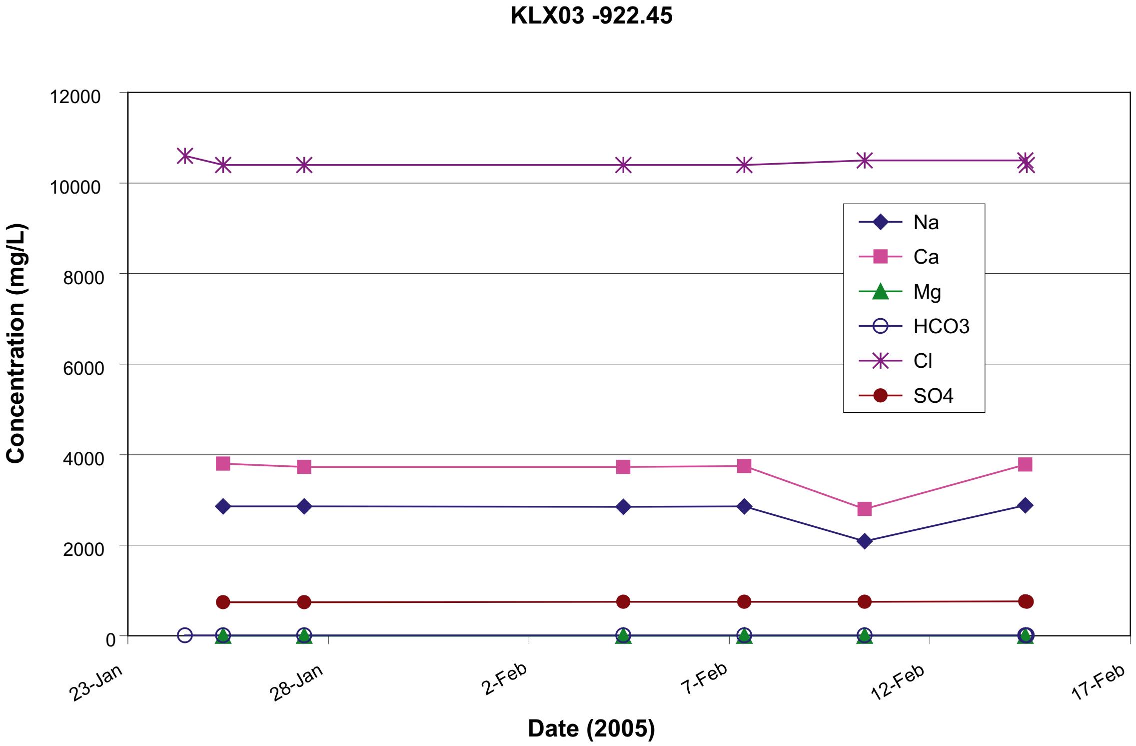
ID CODE	SAMPLE DATE	ELEVATION (MID)	COMMENTS	CLASS NO	Drilling water residue (%)	pH (lab)	Electric Conductivity (mS/m)	SEC UP (m)	SEC LOW (m)	Relative charge balance (%) from SICADA
HLX14	11/4/2006	–42.17	drill water used for KLX03, KLX13A, KLX15A, KLX17A	3	0.05	7.97	156.0	11.90	115.90	–2.75
HLX14	5/7/2004	–42.17		5		8.11	87.9	11.90	115.90	–1.91
HLX10	3/12/2003	–27.86	drill water used for KLX08	3	0.02	8.23	38.7	0.00	85.00	0.66
HLX10	2/1/2005	–29.25		T4	0.24	8.25	54.0	3.00	85.00	–0.44
HLX10	10/28/2005	–29.25		4	–	7.03	57.0	3.00	85.00	–1.57

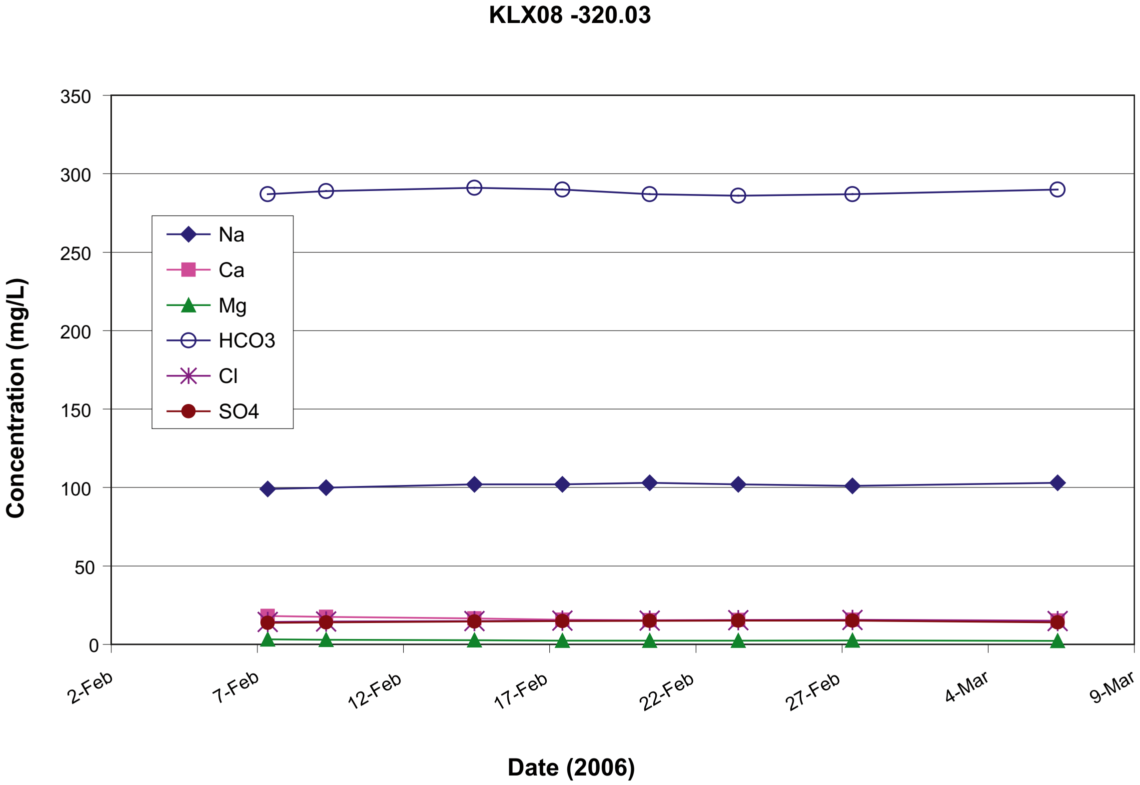
Na	K	Ca	Mg	HCO3	Cl	SO4	Br	Fe	Fe TOT	Fe2+	Sr	H–2 (‰)	Tritium (TU)	O–18 (‰)	C–14 (pmc)	S–34 (‰)	Sr–87/ Sr–86	TOC (mg/L)
248.0	5.35	44.1	12.9	223.00	357.0	53.60	1.290	0.3620			0.844	–84.4	2.50	–11.20	49.70	26.9		
138.0	3.08	18.8	4.7	302.00	69.7	31.30	0.415	0.2690			0.320	–78.6	3.80	–11.20	54.70	32.1	0.715656	7.8
67.7	2.81	12.9	4.4	198.00	6.3	17.84	–0.200	0.0975			0.116	–78.8	7.20	–10.90	55.73	16.2	0.715828	2.90
105.0	3.55	11.8	3.9	221.00	29.1	46.30	–0.200	0.1010			0.111	–75.0	5.20	–10.90	51.72	16.9	0.715733	5.50
104.0	3.19	11.9	4.1	219.00	31.9	49.20	0.313	0.0997	–	–	0.101	–76.9	5.70	–10.80	52.73	16.4	0.715710	5.80

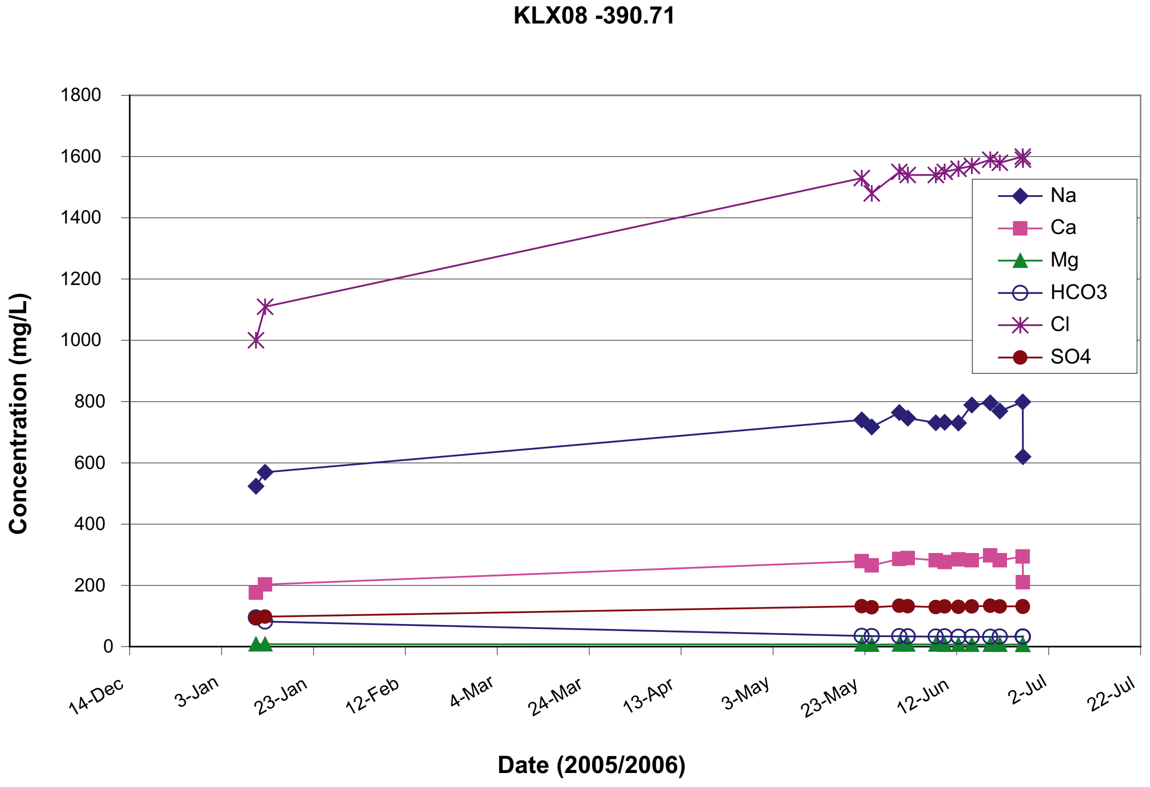
Plots of ion concentrations against date of sampling for 10 sections of Laxemar boreholes.

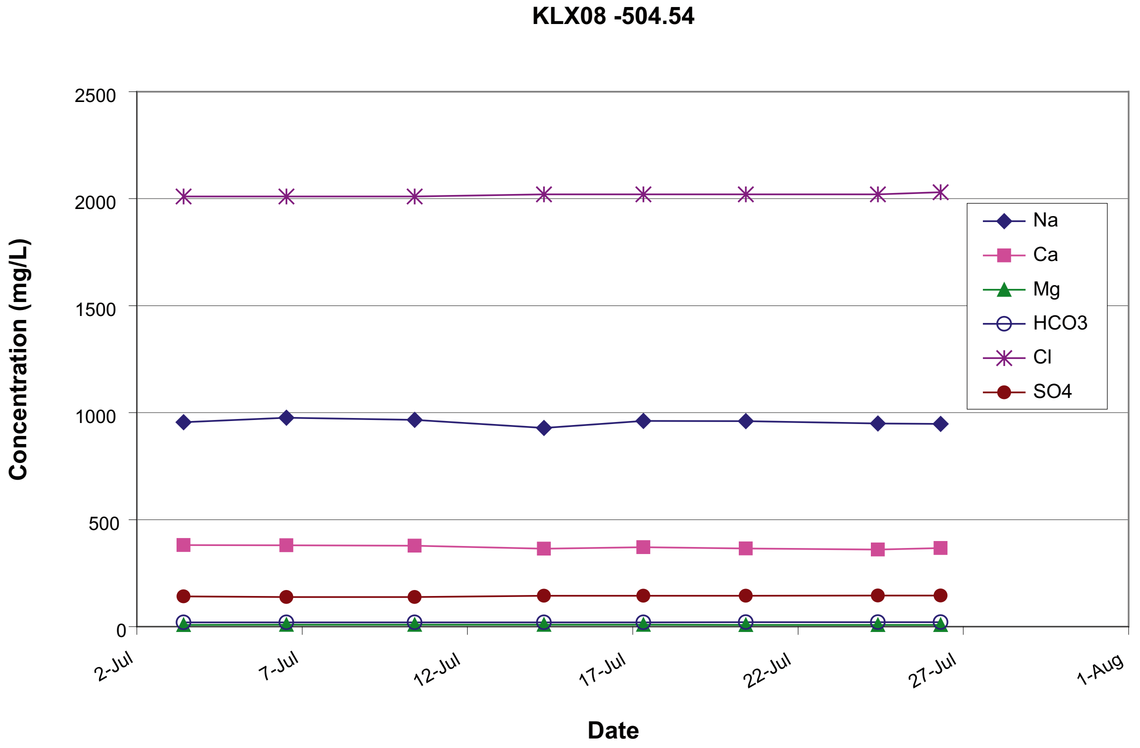




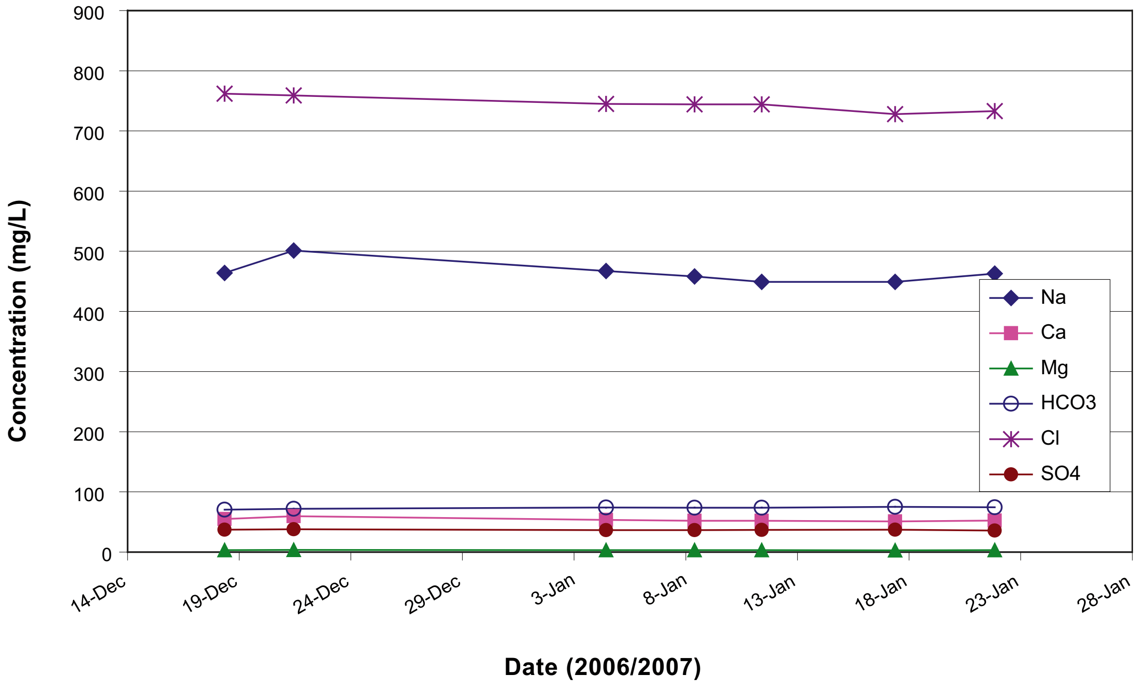

KLX03 -922.45
Concentration (mg/L)
12000
10000
8000
6000
4000
2000
0
23-Jan
28-Jan
2-Feb
7-Feb
12-Feb
17-Feb
Date (2005)
Na
Ca
Mg
HCO3
Cl
SO4


KLX08 -320.03
Concentration (mg/L)
350
300
250
200
150
100
50
0
2-Feb
7-Feb
12-Feb
17-Feb
22-Feb
27-Feb
4-Mar
9-Mar
Date (2006)
Na
Ca
Mg
HCO3
Cl
SO4

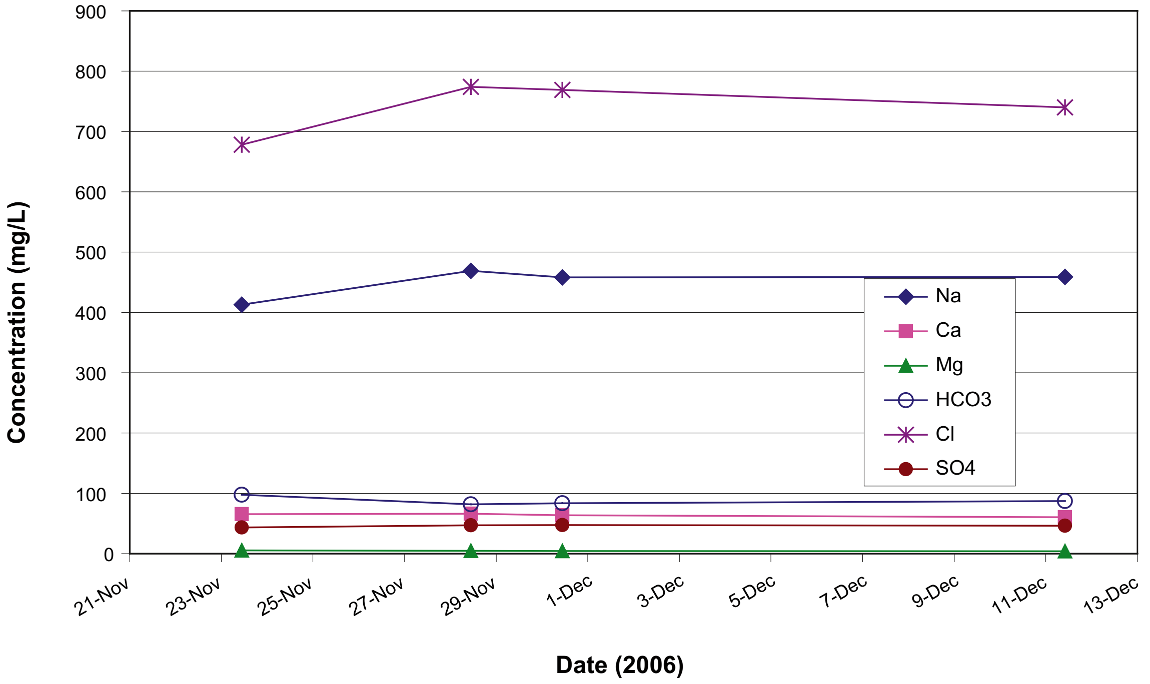

KLX08 -390.71
Concentration (mg/L)
1800
1600
1400
1200
1000
800
600
400
200
0
14-Dec
3-Jan
23-Jan
12-Feb
4-Mar
24-Mar
13-Apr
3-May
23-May
12-Jun
2-Jul
22-Jul
Date (2005/2006)
Na
Ca
Mg
HCO3
Cl
SO4

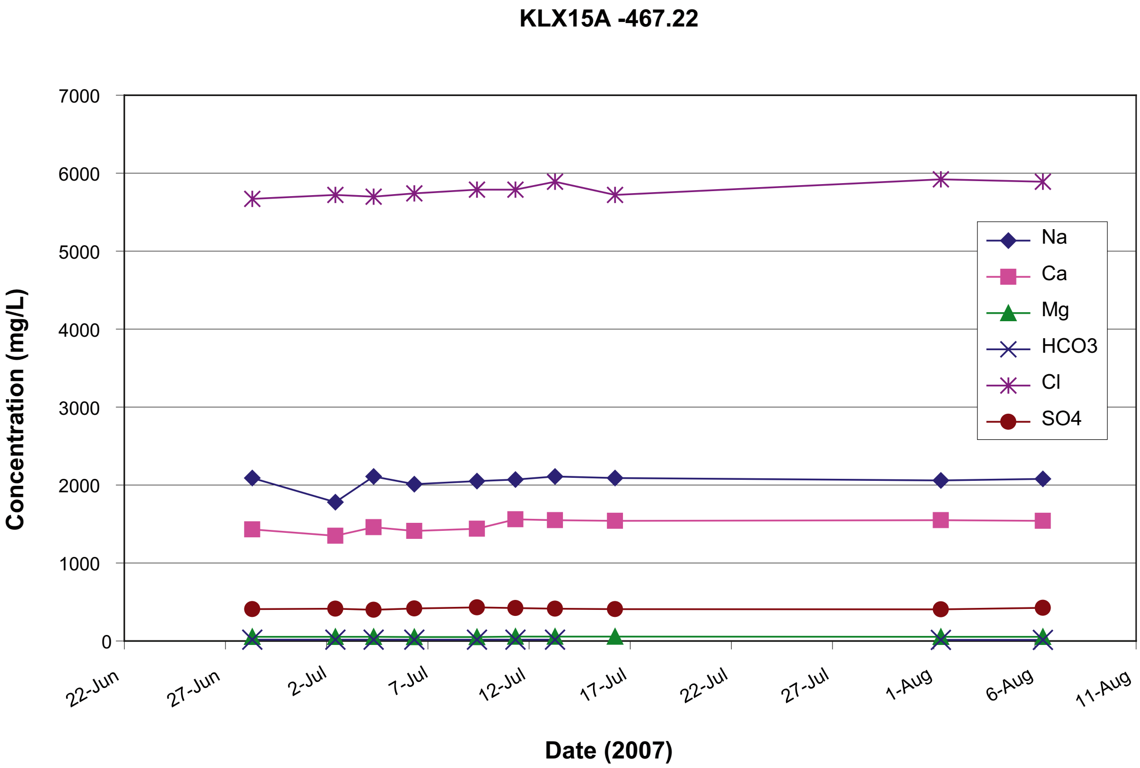

KLX08 -504.54
Concentration (mg/L)
2500
2000
1500
1000
500
0
2-Jul
7-Jul
12-Jul
17-Jul
22-Jul
27-Jul
1-Aug
Date
Na
Ca
Mg
HCO3
Cl
SO4

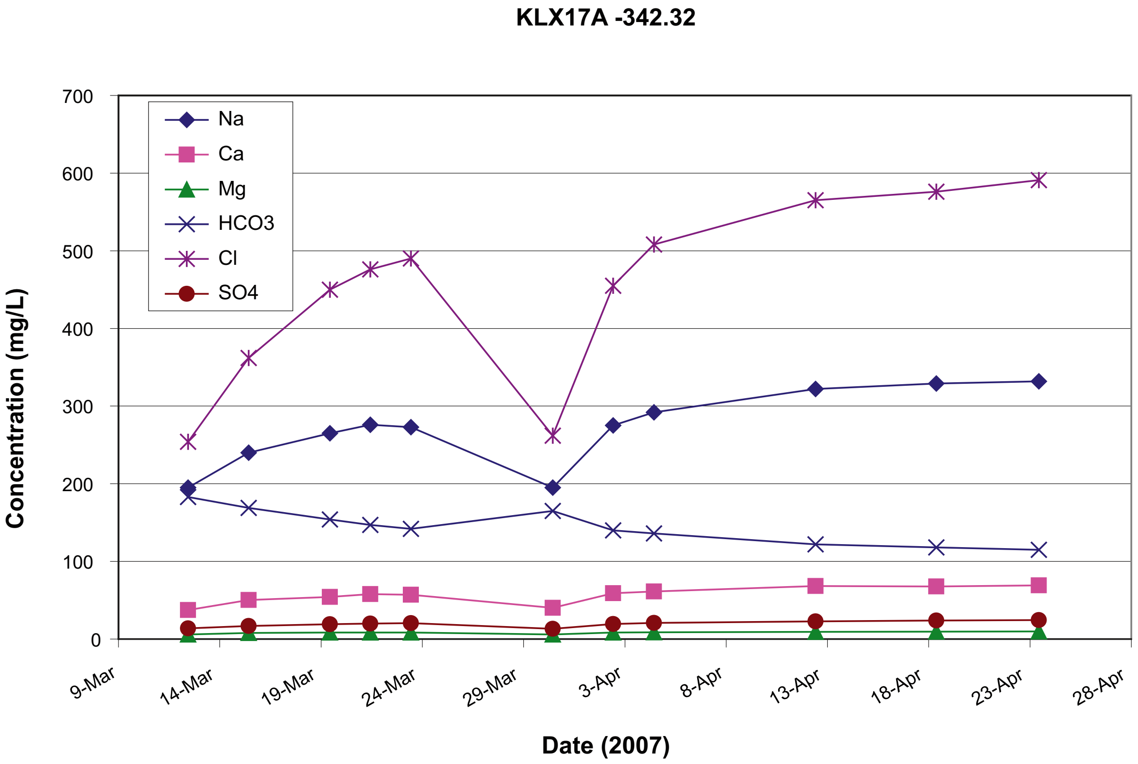
KLX13A -408.01



KLX13A -474.99

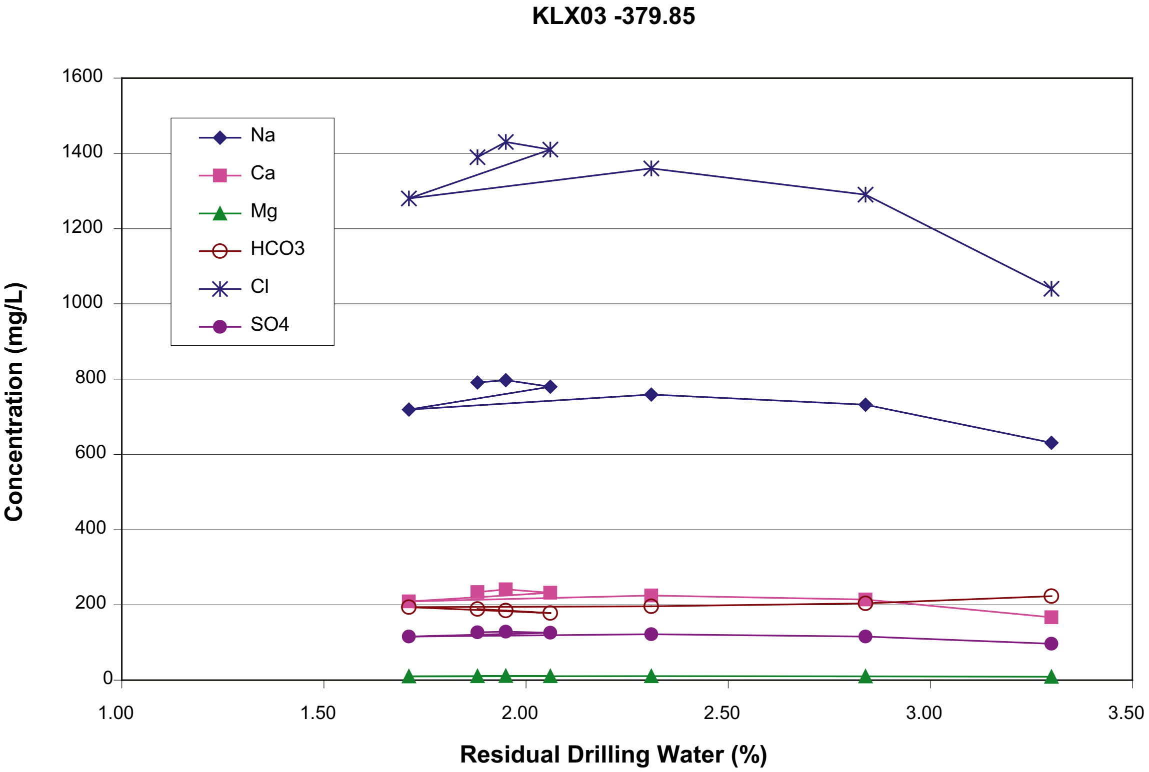


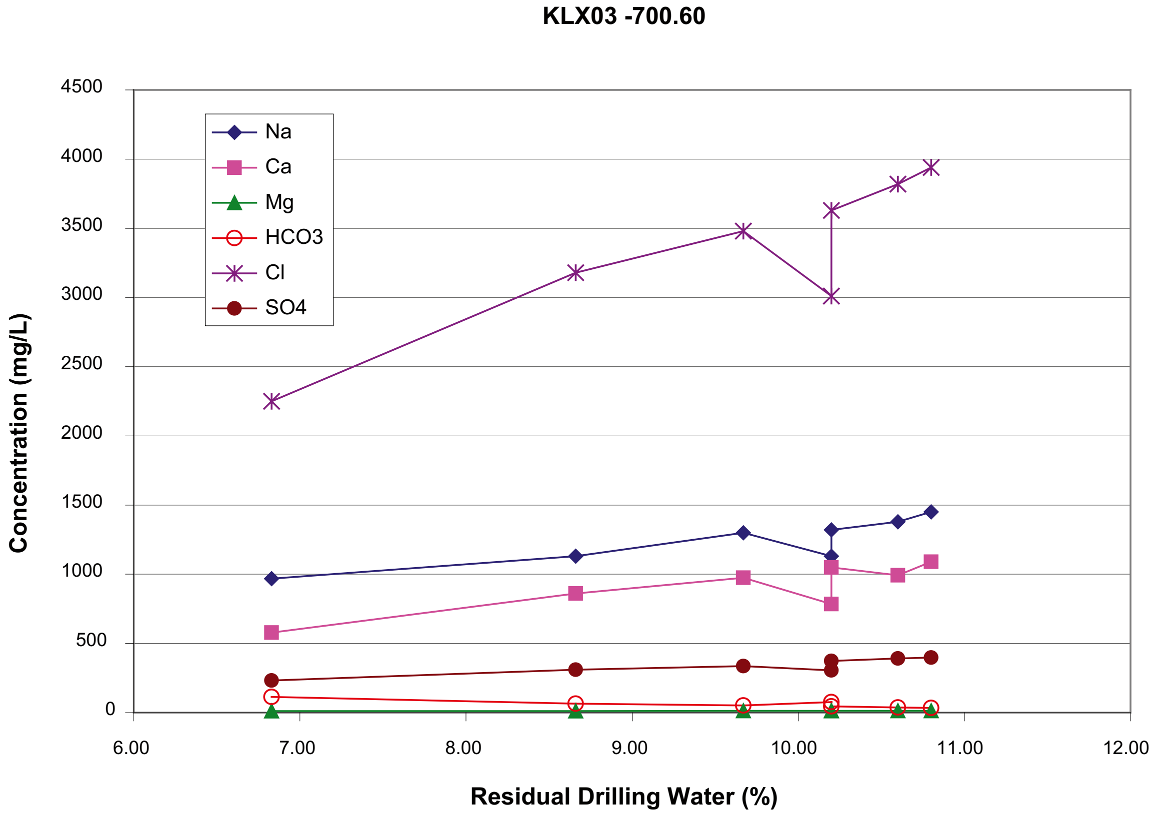

KLX15A -467.22
Concentration (mg/L)
7000
6000
5000
4000
3000
2000
1000
0
22-Jun
27-Jun
2-Jul
7-Jul
12-Jul
17-Jul
22-Jul
27-Jul
1-Aug
6-Aug
11-Aug
Date (2007)
Na
Ca
Mg
HCO3
Cl
SO4

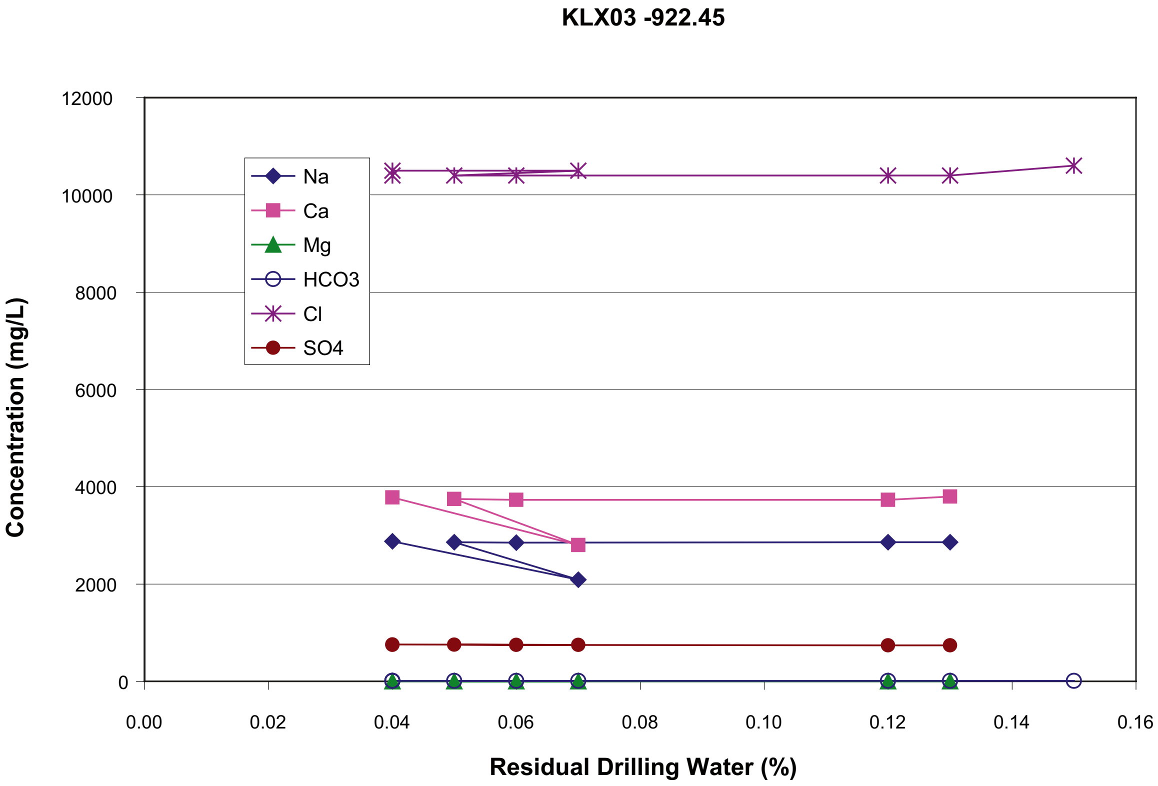

KLX17A -342.32
Concentration (mg/L)
700
600
500
400
300
200
100
0
9-Mar
14-Mar
19-Mar
24-Mar
29-Mar
3-Apr
8-Apr
13-Apr
18-Apr
23-Apr
28-Apr
Date (2007)
Na
Ca
Mg
HCO3
Cl
SO4

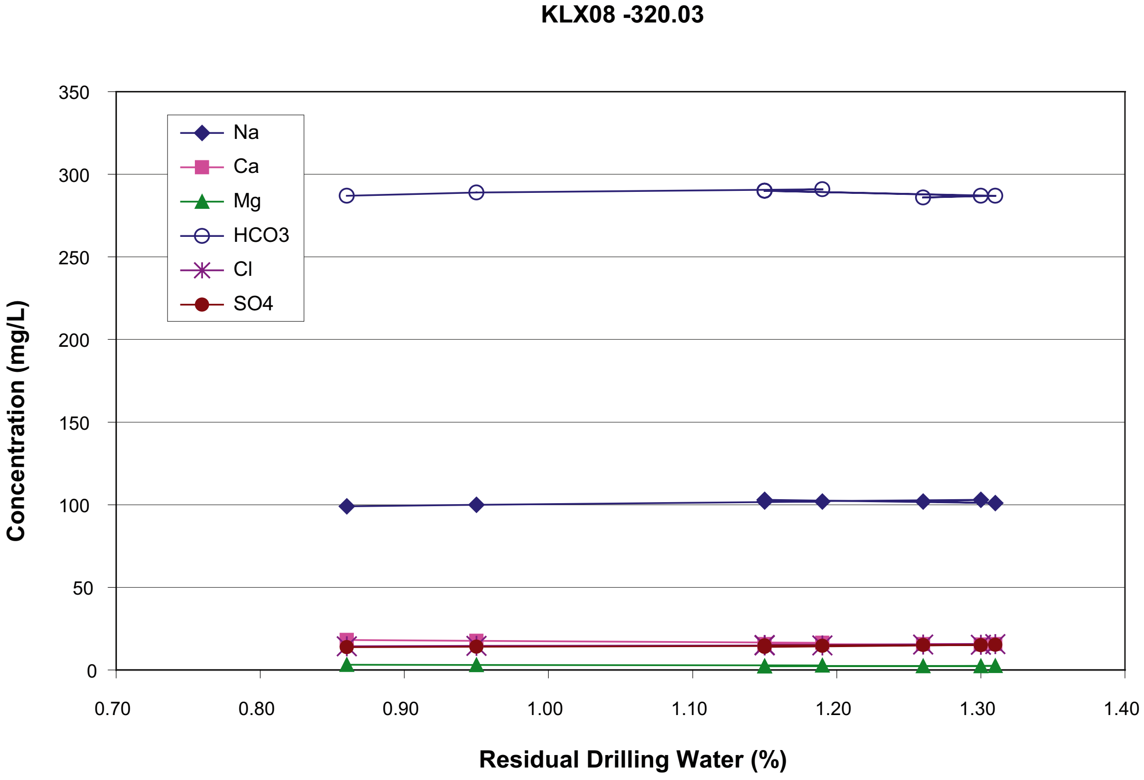
Appendix 4

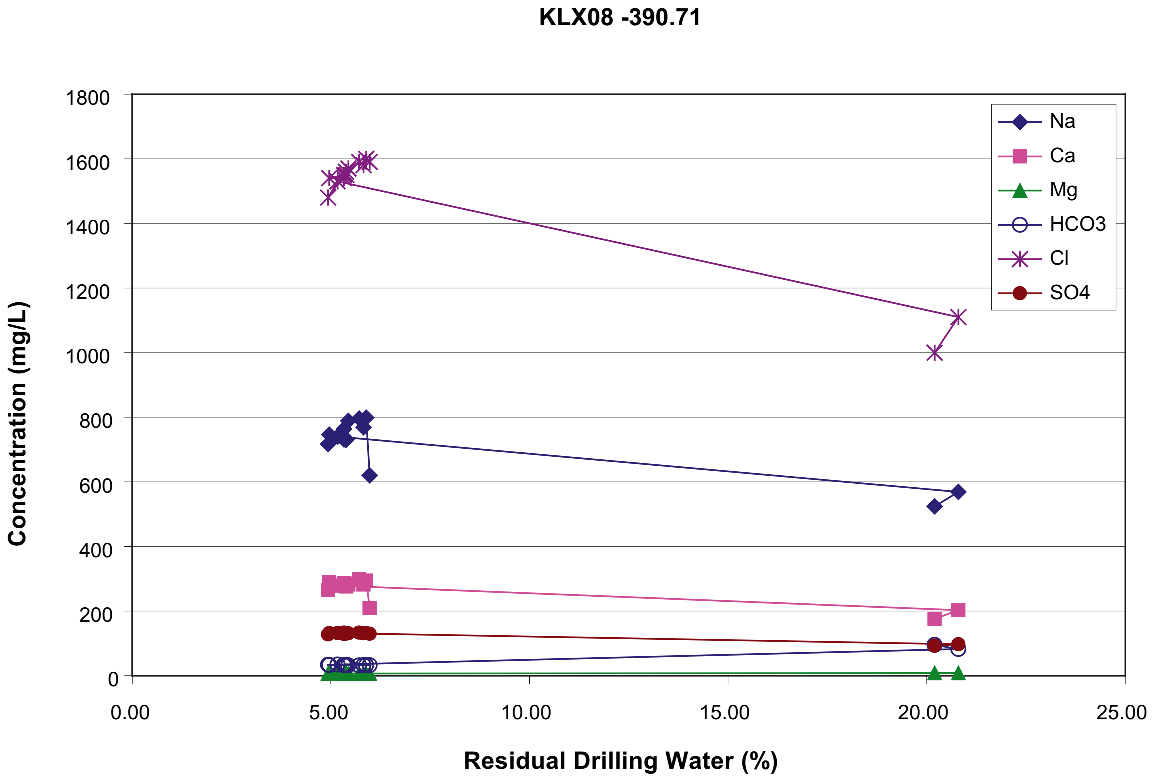
Plots of ion concentrations against percent of residual drill water in 10 sections of Laxemar boreholes.

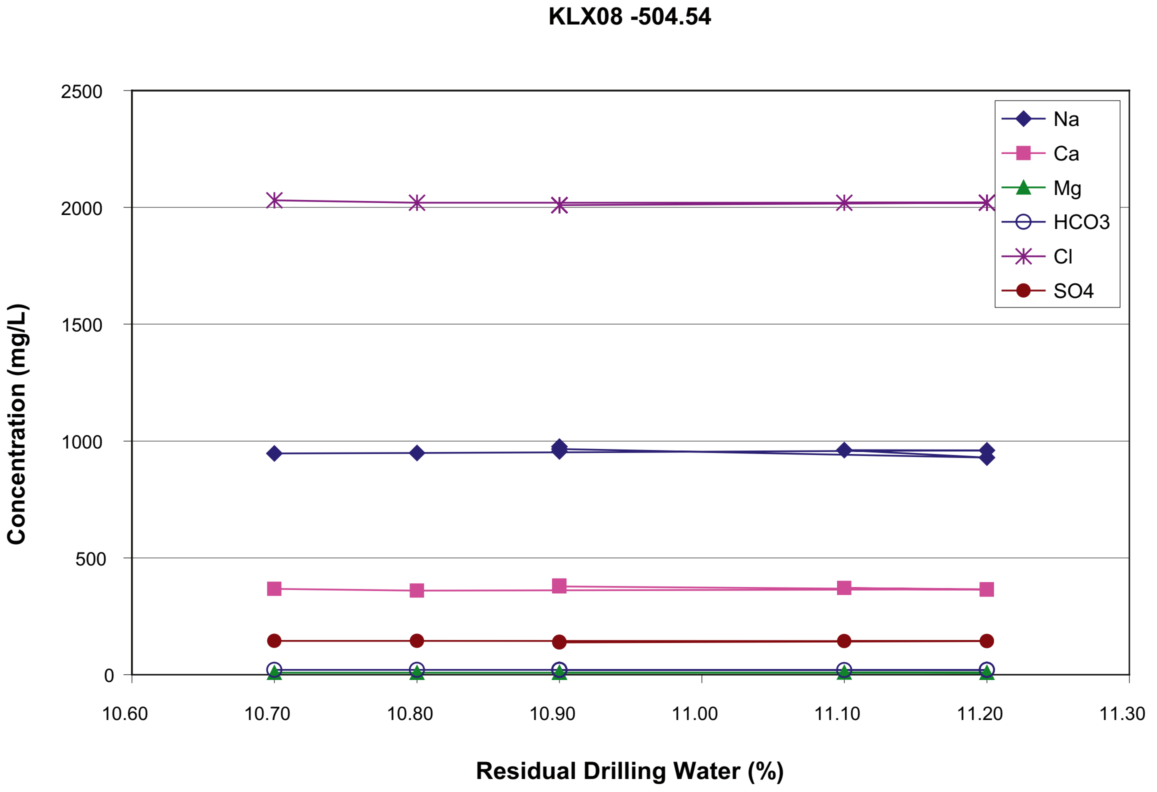


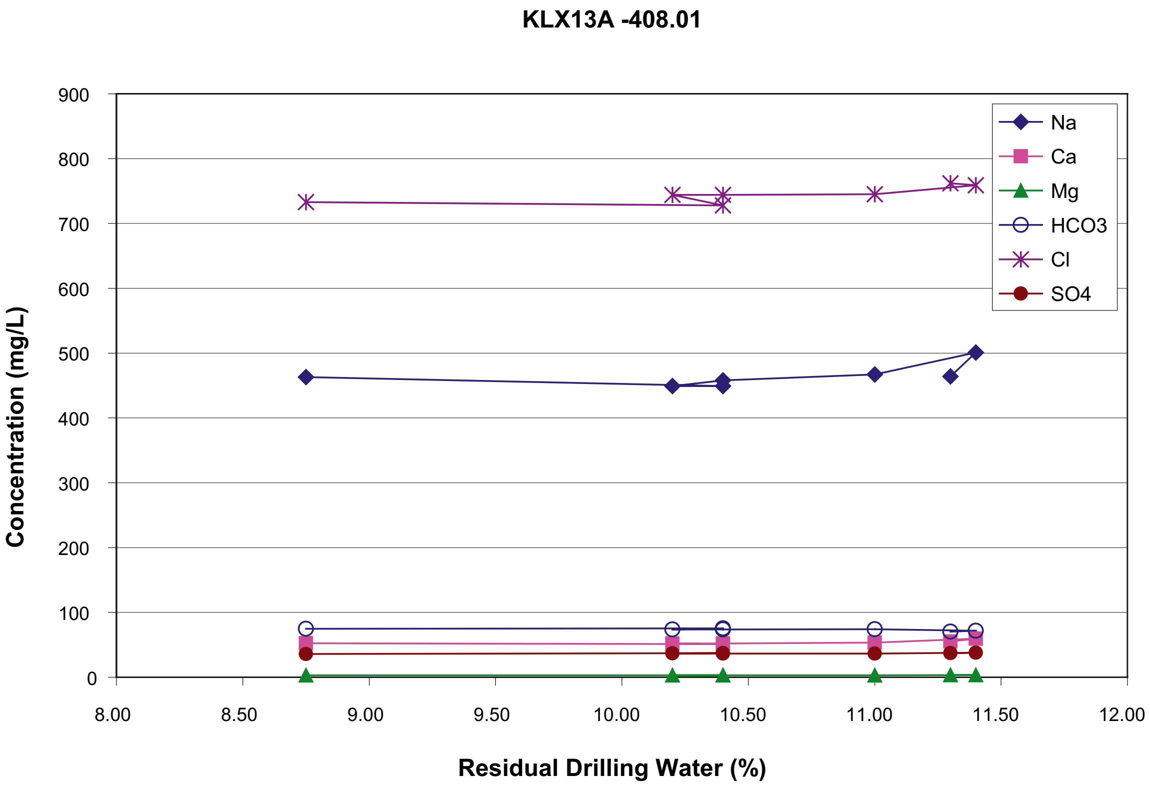


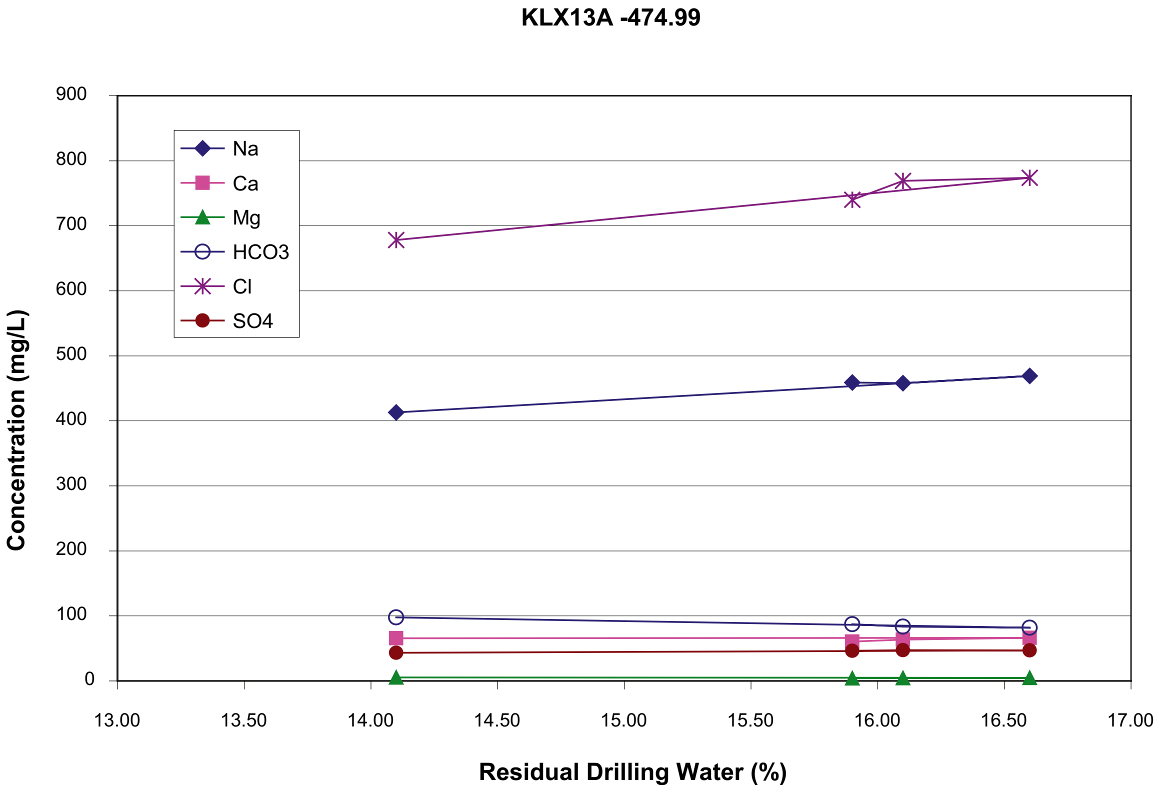

KLX03 -922.45
Concentration (mg/L)
Residual Drilling Water (%)
0
2000
4000
6000
8000
10000
12000
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0.16
Na
Ca
Mg
HCO3
Cl
SO4

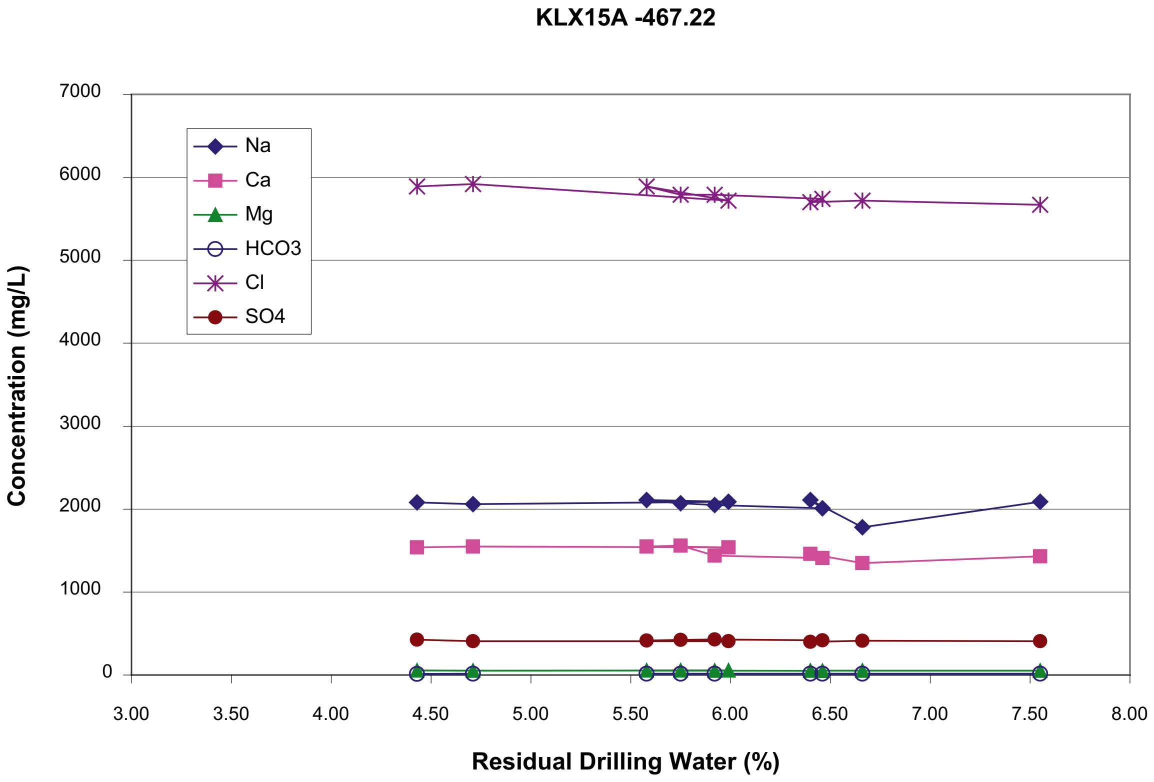

KLX08 -320.03
Concentration (mg/L)
Residual Drilling Water (%)
0
50
100
150
200
250
300
350
0.70
0.80
0.90
1.00
1.10
1.20
1.30
1.40
Na
Ca
Mg
HCO3
Cl
SO4

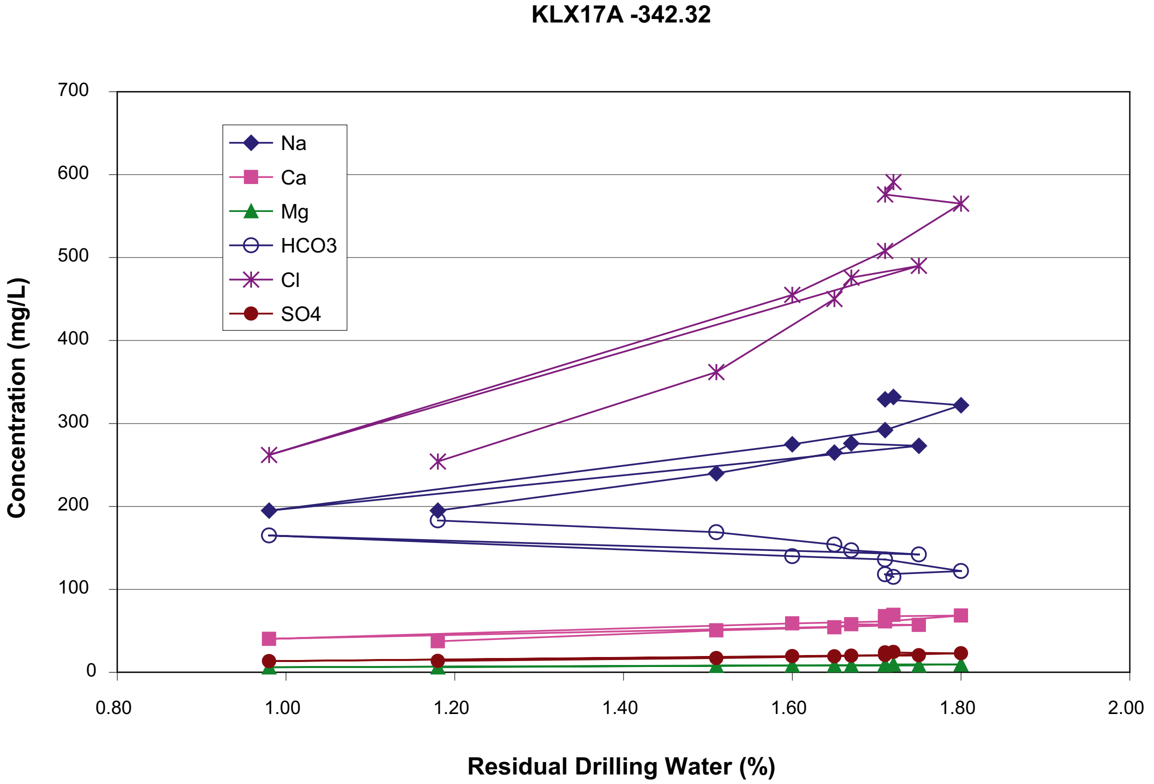

KLX08 -390.71


KLX08 -504.54


KLX13A -408.01
Concentration (mg/L)
900
800
700
600
500
400
300
200
100
0
8.00
8.50
9.00
9.50
10.00
10.50
11.00
11.50
12.00
Residual Drilling Water (%)
Na
Ca
Mg
HCO3
Cl
SO4

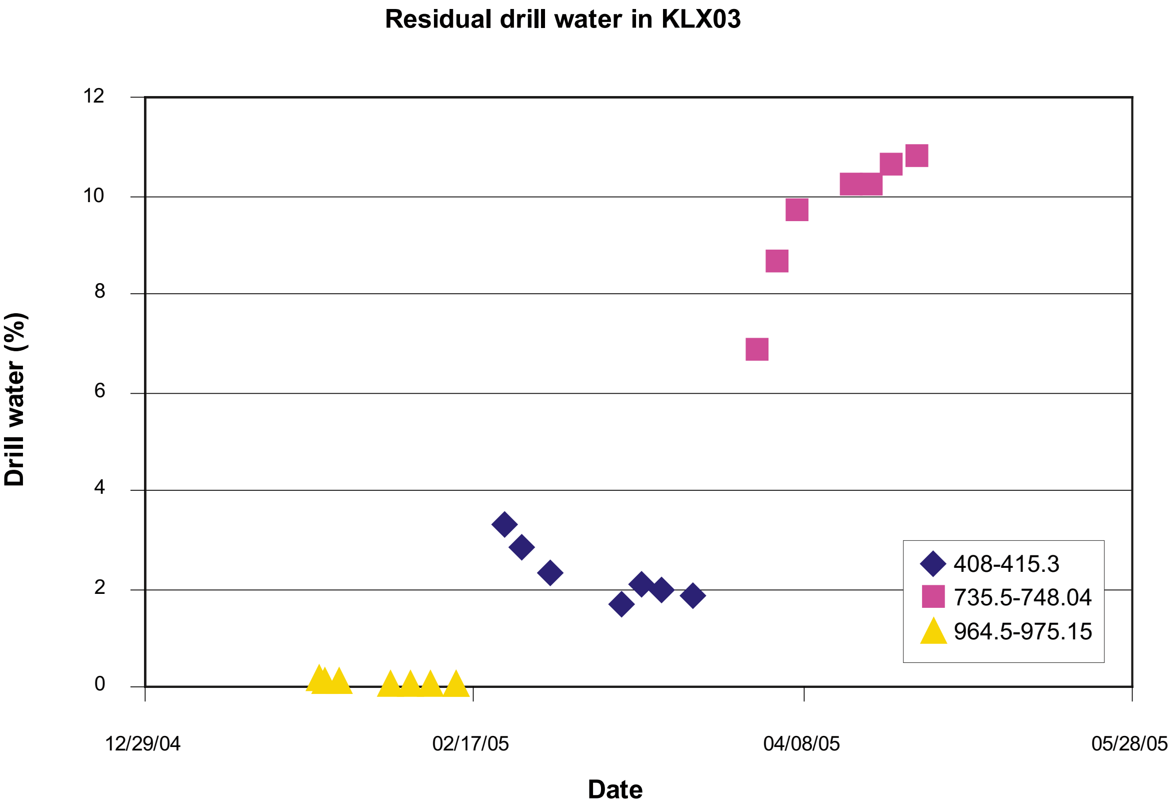

KLX13A -474.99
Concentration (mg/L)
900
800
700
600
500
400
300
200
100
0
13.00
13.50
14.00
14.50
15.00
15.50
16.00
16.50
17.00
Residual Drilling Water (%)
Na
Ca
Mg
HCO3
Cl
SO4

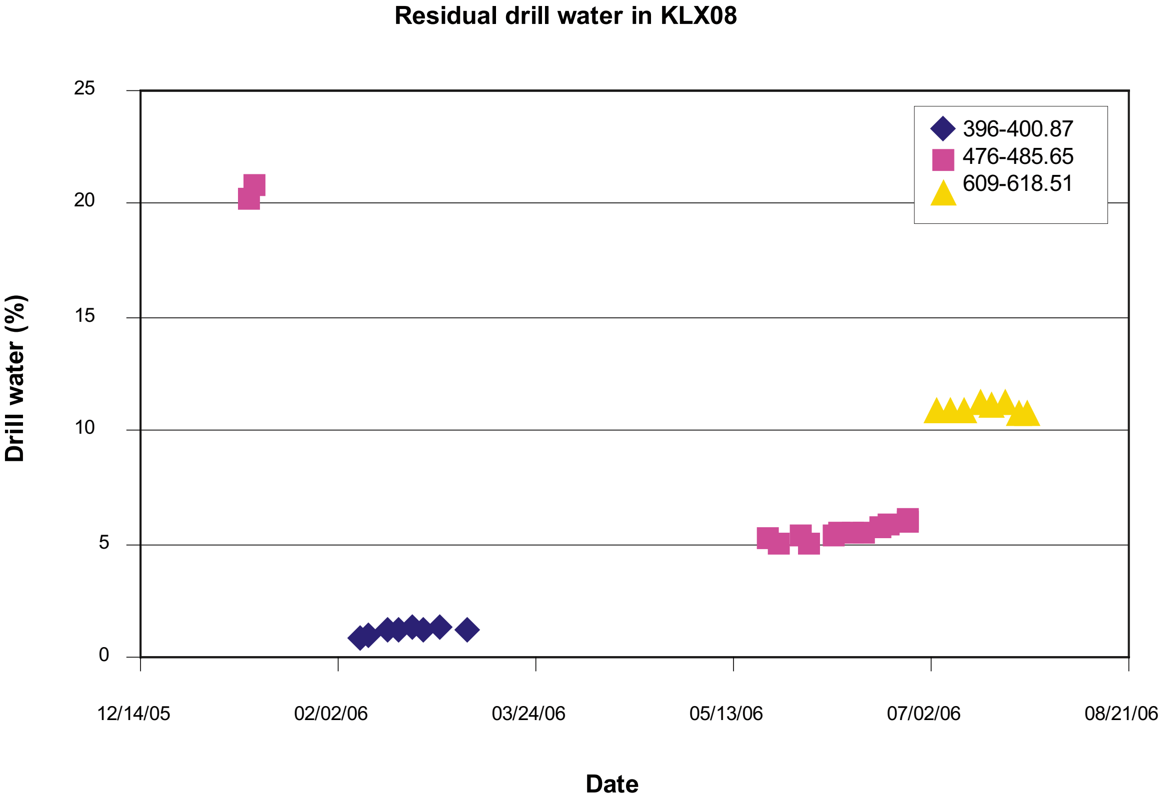

KLX15A -467.22
Concentration (mg/L)
7000
6000
5000
4000
3000
2000
1000
0
3.00
3.50
4.00
4.50
5.00
5.50
6.00
6.50
7.00
7.50
8.00
Residual Drilling Water (%)
Na
Ca
Mg
HCO3
Cl
SO4


KLX17A -342.32
Concentration (mg/L)
700
600
500
400
300
200
100
0
0.80
1.00
1.20
1.40
1.60
1.80
2.00
Residual Drilling Water (%)
Na
Ca
Mg
HCO3
Cl
SO4

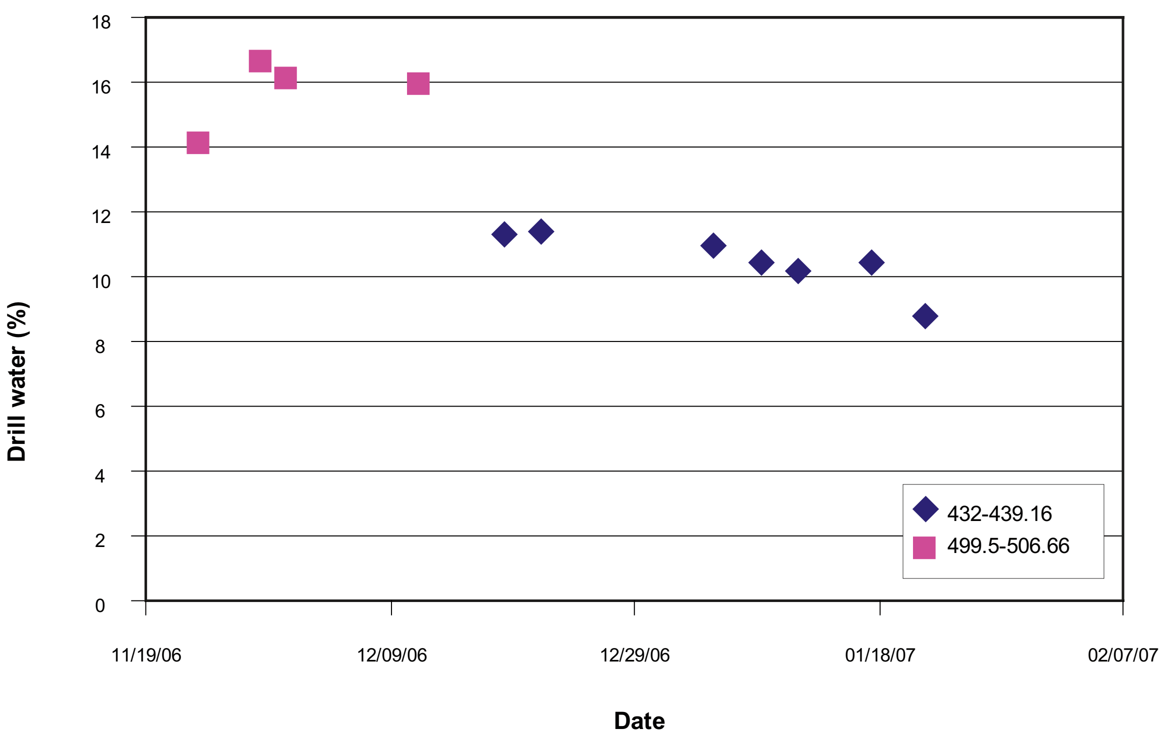
Appendix 5

Plots of percent residual drill water against date in 10 sections of Laxemar boreholes.

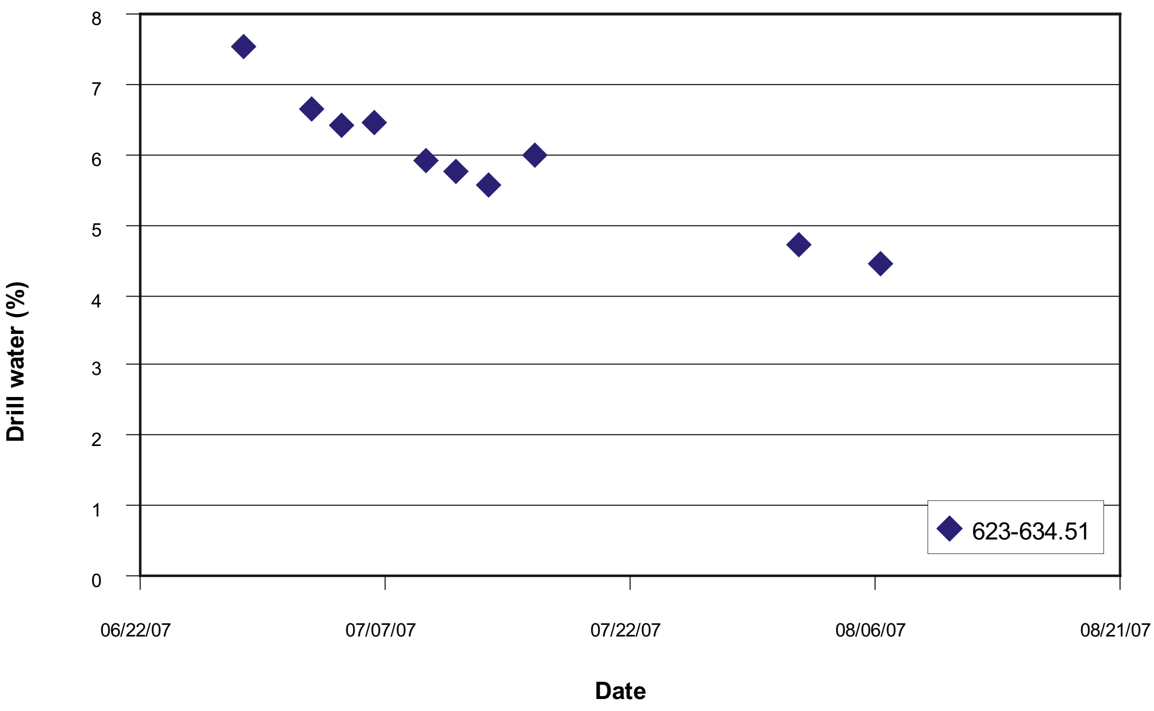


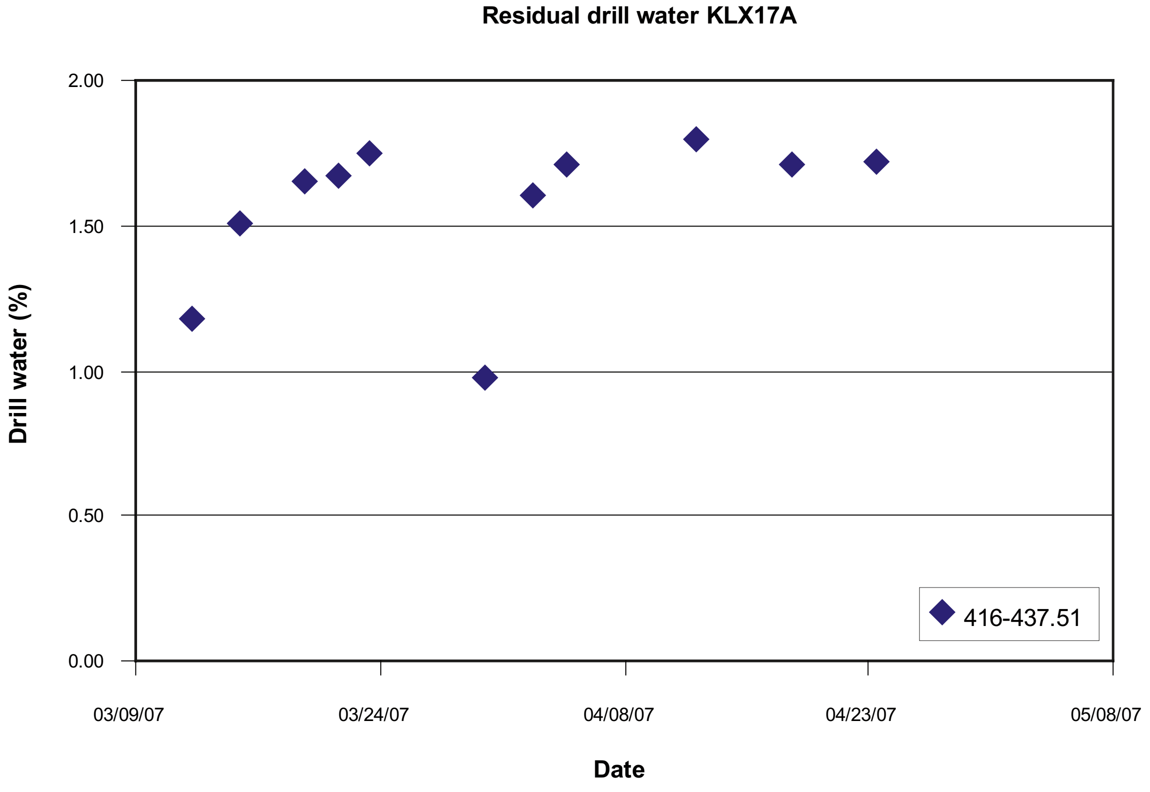


Residual drill water in KLX13A



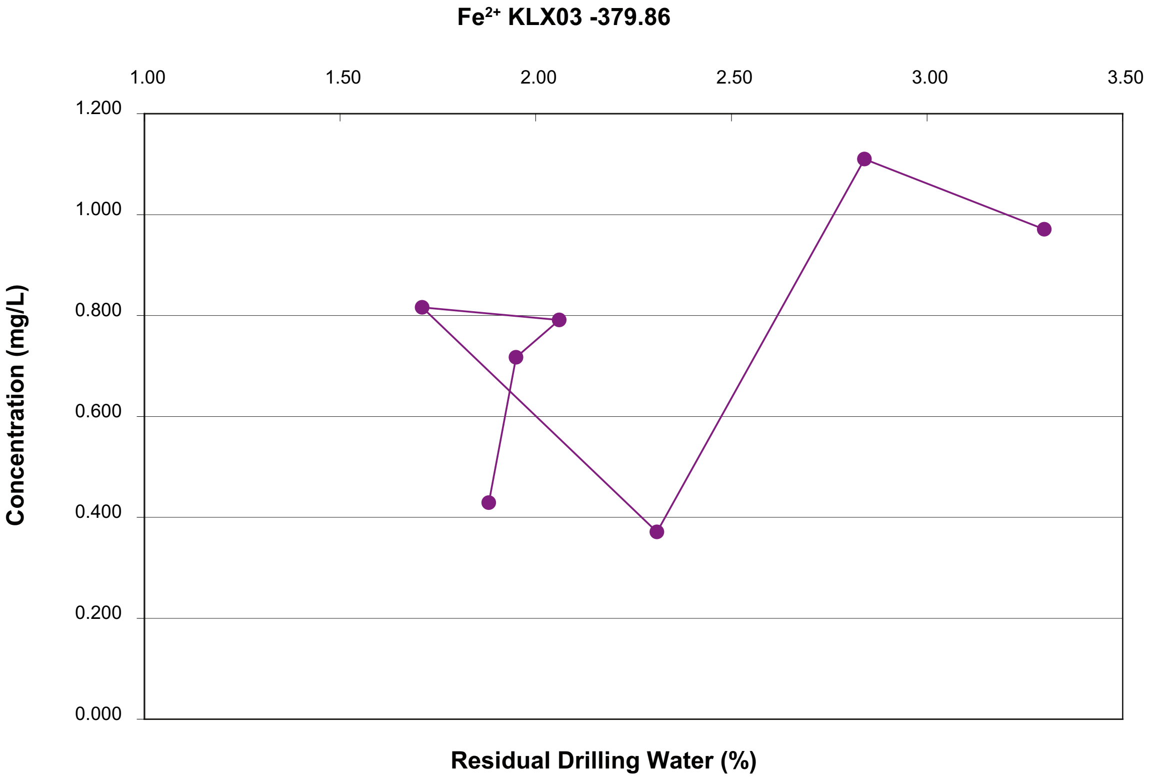
Residual drill water in KLX15A

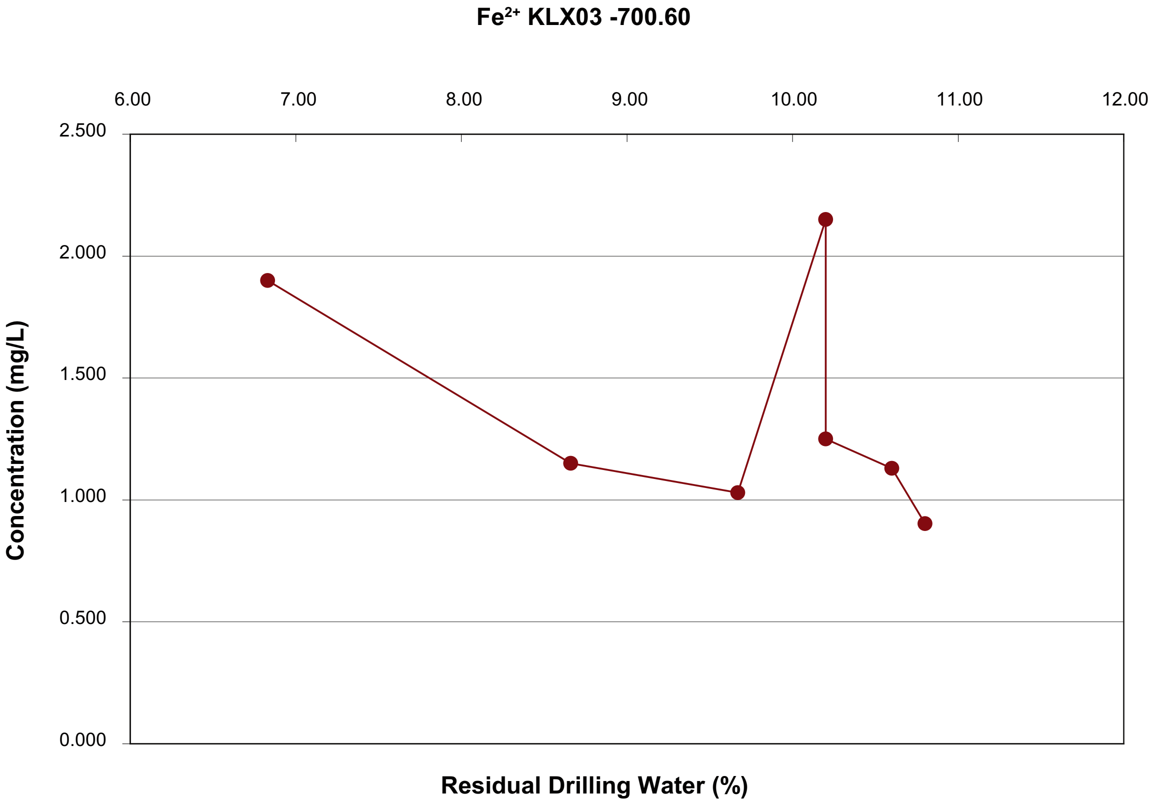


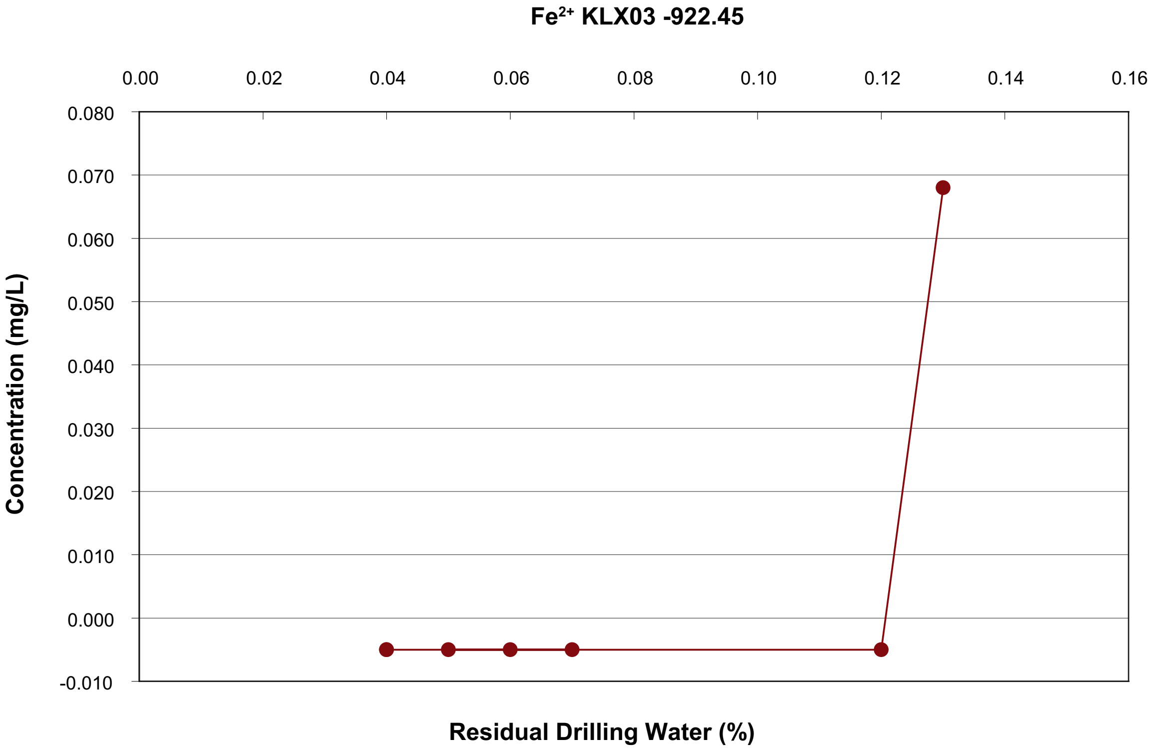

Residual drill water KLX17A
Drill water (%)
2.00
1.50
1.00
0.50
0.00
03/09/07
03/24/07
04/08/07
04/23/07
05/08/07
Date
416-437.51

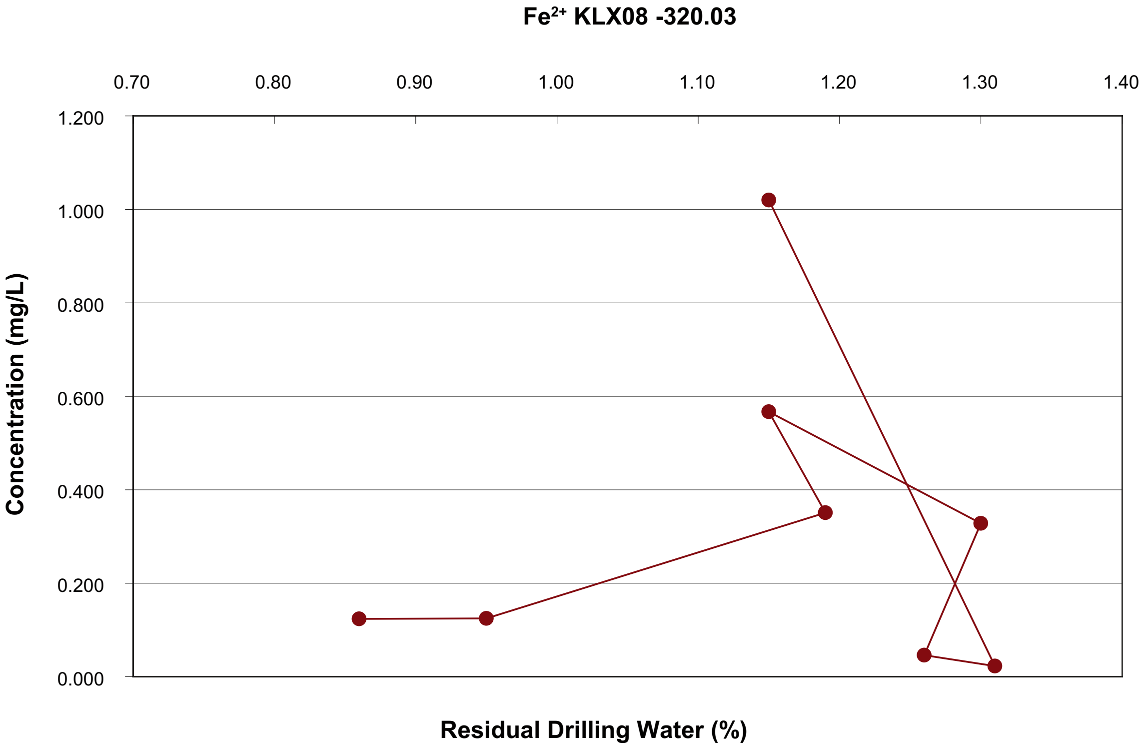
Appendix 6

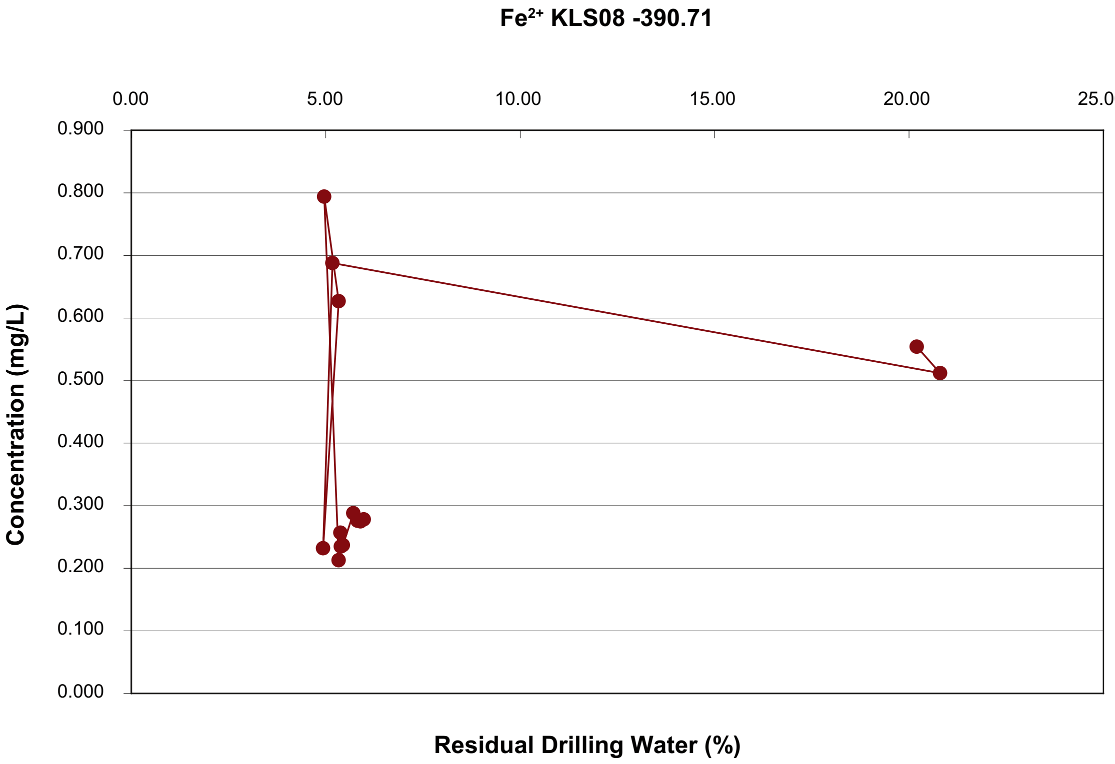
Plots of iron (Fe^{2+}) concentrations against percent of residual drill water in 10 sections of Laxemar boreholes.

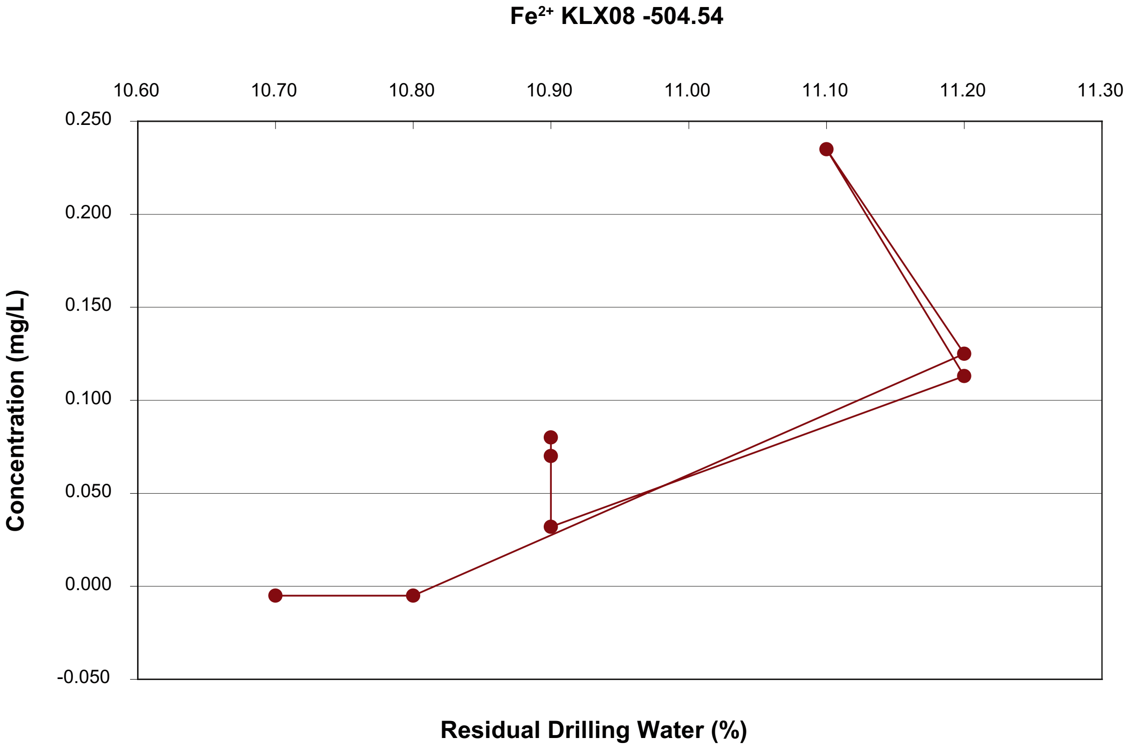


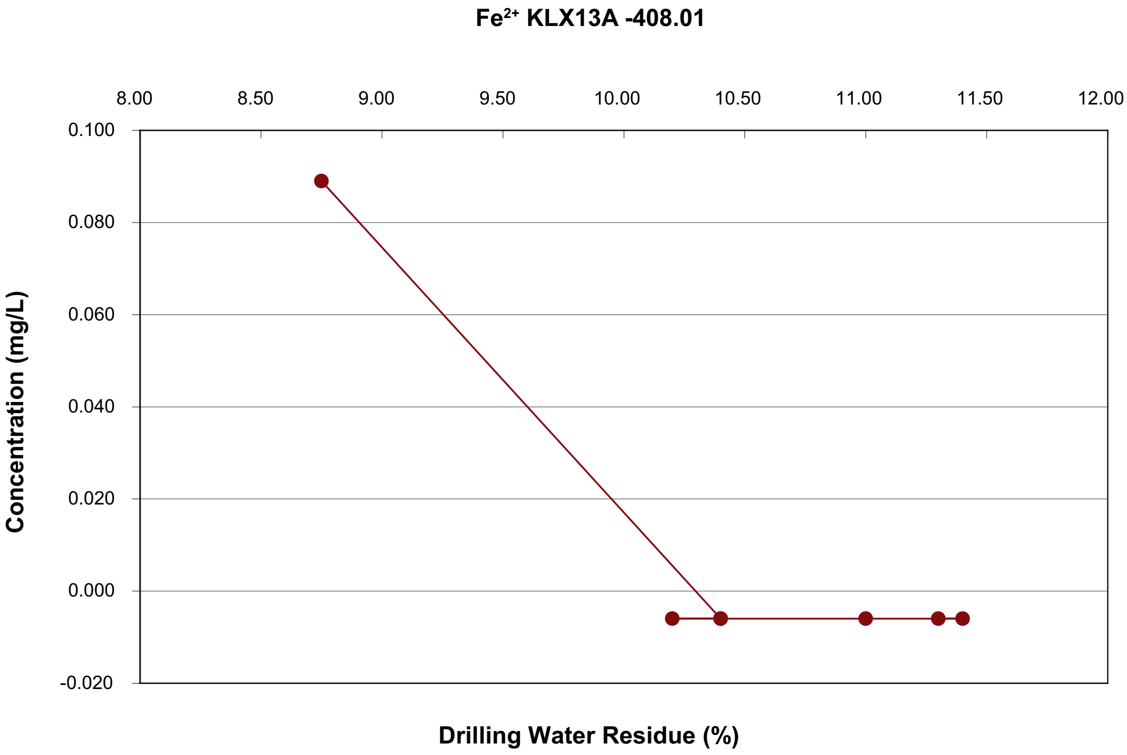


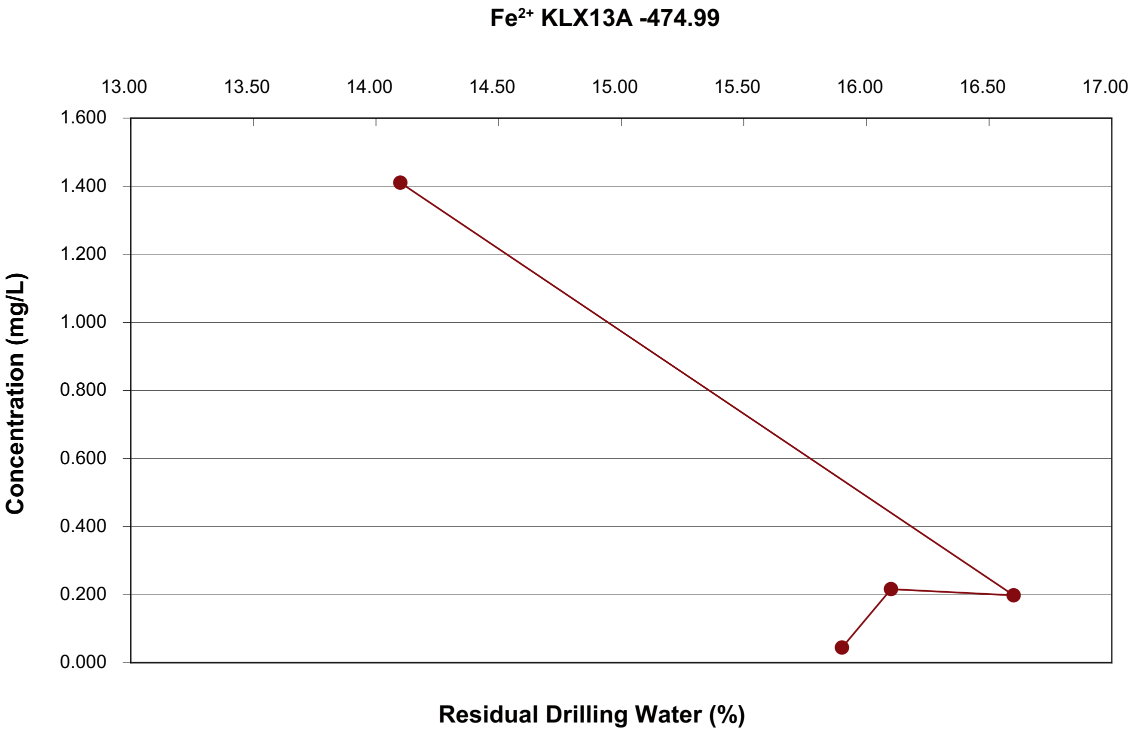

Fe²⁺ KLX03 -922.45
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0.16
0.080
0.070
0.060
0.050
0.040
0.030
0.020
0.010
0.000
-0.010
Concentration (mg/L)
Residual Drilling Water (%)

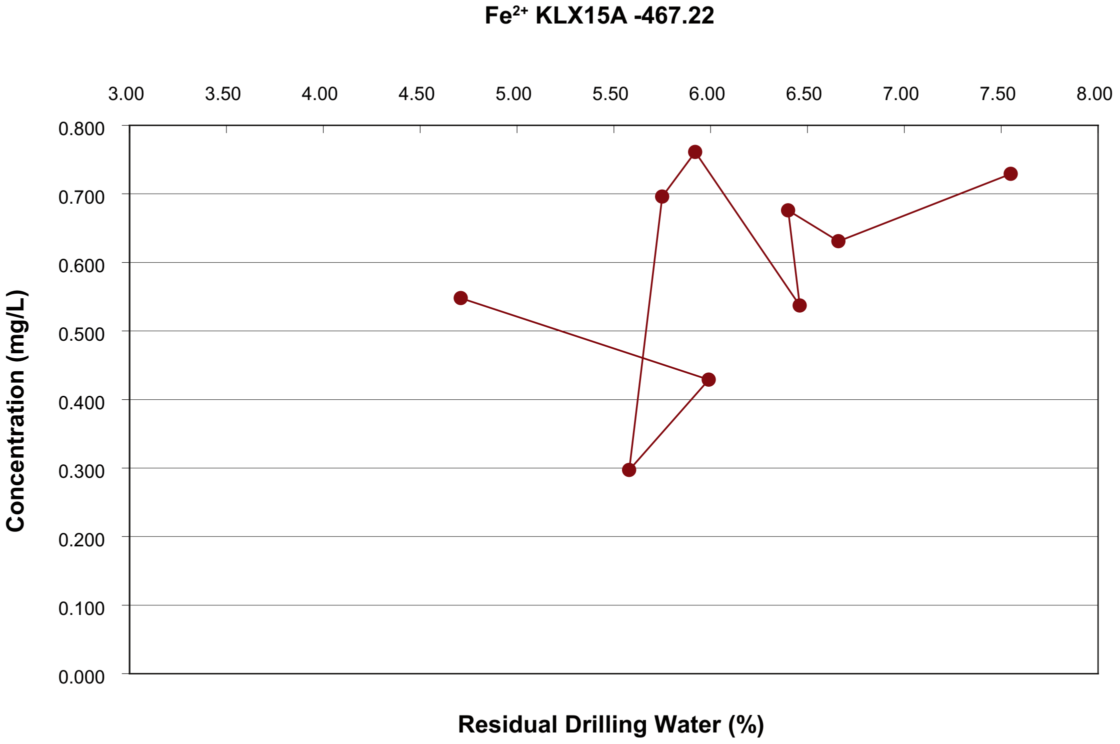

Fe²⁺ KLX08 -320.03
0.70
0.80
0.90
1.00
1.10
1.20
1.30
1.40
1.200
1.000
0.800
0.600
0.400
0.200
0.000
Concentration (mg/L)
Residual Drilling Water (%)

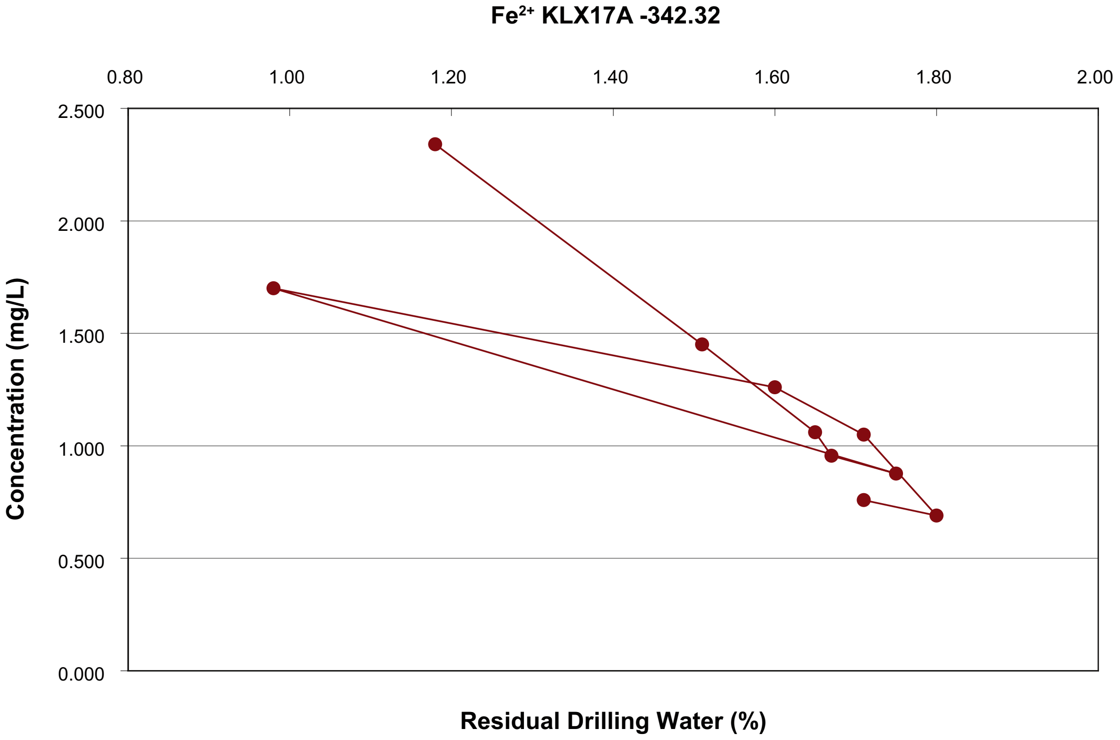

Fe^{2+} KLS08 -390.71
0.00
5.00
10.00
15.00
20.00
25.00
0.900
0.800
0.700
0.600
0.500
0.400
0.300
0.200
0.100
0.000
Concentration (mg/L)
Residual Drilling Water (%)


Fe^{2+} KLX08 -504.54
10.60
10.70
10.80
10.90
11.00
11.10
11.20
11.30
0.250
0.200
0.150
0.100
0.050
0.000
-0.050
Concentration (mg/L)
Residual Drilling Water (%)


Fe²⁺ KLX13A -408.01
8.00
8.50
9.00
9.50
10.00
10.50
11.00
11.50
12.00
0.100
0.080
0.060
0.040
0.020
0.000
-0.020
Concentration (mg/L)
Drilling Water Residue (%)


Fe²⁺ KLX13A -474.99
13.00
13.50
14.00
14.50
15.00
15.50
16.00
16.50
17.00
1.600
1.400
1.200
1.000
0.800
0.600
0.400
0.200
0.000
Concentration (mg/L)
Residual Drilling Water (%)


Fe²⁺ KLX15A -467.22
3.00
3.50
4.00
4.50
5.00
5.50
6.00
6.50
7.00
7.50
8.00
0.800
0.700
0.600
0.500
0.400
0.300
0.200
0.100
0.000
Concentration (mg/L)
Residual Drilling Water (%)


Fe²⁺ KLX17A -342.32
0.80
1.00
1.20
1.40
1.60
1.80
2.00
2.500
2.000
1.500
1.000
0.500
0.000
Concentration (mg/L)
Residual Drilling Water (%)

Section 4

Laxemar site investigation
Quality of hydrochemical analyses (DF version 2.3)

Ann-Chatrin Nilsson
Geosigma AB

Contents

1 Introduction

The hydrochemical data generated from the site investigation programme in Laxemar constitute the following four types:

1. Data from chemical analyses.
2. Data from long-term on-line measurements in flow-through cells (Chemmac measurements).
3. Data from field measurements of surface waters and near-surface groundwaters.
4. Special studies or experiments.

This quality evaluation assesses the chemical analyses performed by SKB (Äspö chemical laboratory) and by contracted external laboratories. Analytical methods and reported measurement uncertainties are presented in Chapter 2. A detailed description concerning sampling methods, sample preparation and analytical methods is given in /Nilsson 2005/.

The discussions in this document focus on some selected constituents of particular importance for hydrochemical interpretations and modelling as well as on methods/constituents that have been questioned or are known, from experience, to be somewhat unreliable.

Of first concern, when interpreting the hydrogeochemical data, is contamination by drilling water in the groundwater samples. Not only the reliability of the uranine analyses (the dye used to trace the drilling water) and the size of the analytical errors, but also other conditions affect the confidence in the drilling water budget calculations, the drilling water contents in water samples and, indirectly, the judgement of sample quality/representativity.

Second, there is a need to establish a consistent set of major constituent concentrations for each sample and those ions with high enough concentration to affect the charge balance were considered (mainly Na, Ca, Cl, SO_4 and possibly Mg and HCO_3).

Of fundamental importance is also the reliability of data for constituents and parameters that are indicators of groundwater origin like oxygen-18 and of marine contributions (Littorina sea water) like magnesium and bromide. Furthermore, reliable data is crucial for constituents and parameters that are of importance in order to understand redox conditions such as iron and sulphide. The sulphide concentration is also a critical parameter for safety assessment evaluations /SKB 2006/.

2 Measurement uncertainties, detection limits and reporting limits

An updated list of analytical methods, reporting limits and general measurement uncertainties as reported from the contracted laboratories at present is displayed in Table 2-1. The uncertainties are included as error bars in the diagrams displayed in the following chapters.

Measurement uncertainties were reported as general estimates as well as separate values stated for each reported concentration value. General advance estimates of measurement uncertainties for different components were reported from the contracted laboratories at the start of the site investigations in 2002. Only a few changes/modifications of methods or changes of laboratories have occurred during the site characterisation period. However, despite this, reported general measurement uncertainties have varied from time to time for several constituents. Generally, the uncertainties have increased due to a more critical approach and change of estimation method according to more recently established and internationally accepted methods.

For example, the general measurement uncertainties for different ICP analyses reported after 2005 were about twice as high as the initially reported ones. These extended measurement uncertainties were based not only on standard deviations from repeated measurements but also on contributions from standard solutions, balances, volume measurements etc. They were reported for concentrations ten times and one hundred times the reporting limits and sometimes also for three different salinity ranges (ICP SFMS). The values in Table 2-1 are selected to represent the most relevant bedrock groundwater conditions. However, the major concentrations in groundwaters were often much higher than one hundred times the reporting limit.

For evaluation and modelling purposes, the separate/individual measurement uncertainties as reported for each concentration value were difficult to handle. The data volume is very large and to work with separate uncertainty values would be very time consuming. Furthermore, the Sicada database does not support storage of these separate uncertainties yet and many data software packages for modelling and evaluation purposes lack the possibility to include them. General estimates for each component were more suitable to use. However, the laboratories use somewhat different methods for their estimation. In, for example, some isotope cases the uncertainties are based only on measurement statistics. Some of the uncertainties seem overestimated compared to the observations from trend plots and other consistency checks. These uncertainties might be valid in the case of only one sample but with a large number of samples at hand the certainty increases.

The concentration values were, most often, reported down to the reporting limit (10×std). However, some anion analyses performed by SKB were reported down to the detection limit (3×std) in order to facilitate further interpretations.

Table 2-1. Methods, reporting limits and measurement uncertainties (updated 2008).

Component	Method[1]	Reporting limits (RL), detection limits (DL) or range[2]	Unit	Measurement uncertainty[3]
pH	Potentiometric	3–10	pH unit	± 0.1
EC	Electrical Conductivity meas.	1–150 150–10,000	mS/m	5% 3%
HCO_3	Alkalinity titration	1	mg/L	4%
Cl^-	Mohr- titration	≥ 70	mg/L	5%
Cl^-	IC	0.5–70		8%
SO_4	IC	0.5	mg/L	12%
Br^-	IC	DL 0.2, RL 0.5	mg/L	15%
Br	ICP SFMS	0.001, 0.004, 0.010[4]	mg/L	25%[5]
F^-	IC	DL 0.2, RL 0.5	mg/L	13%
F^-	Potentiometric	DL 0.1, RL 0.2		12%
I^-	ICP SFMS	0.001, 0.004, 0.010[4]	mg/L	25%[5]

Component	Method[1]	Reporting limits (RL), detection limits (DL) or range[2]	Unit	Measurement uncertainty[3]
Na	ICP AES	0.1	mg/L	13%
K	ICP AES	0.4	mg/L	12%
Ca	ICP AES	0.1	mg/L	12%
Mg	ICP AES	0.09	mg/L	12%
S(tot)	ICP AES	0.16	mg/L	12%
Si(tot)	ICP AES	0.03	mg/L	14%
Sr	ICP AES	0.002	mg/L	12%
Li	ICP AES	0.004	mg/L	12.2%
Fe	ICP AES	0.02	mg/L	13.3%[6]
Fe	ICP SFMS	0.0004, 0.002, 0.004[4]	mg/L	20%[6]
Mn	ICP AES	0.003	mg/L	12.1%[5]
Mn	ICP SFMS	0.00003, 0.00004, 0.0001[4]	mg/L	53%[6]
Fe(II), Fe(tot)	Spectrophotometry	DL 0.006, RL 0.02	mg/L	0.005 (0.02–0.05 mg/L) 9% (0.05–1 mg/L) 7% (1–3 mg/L)
HS^-	Spectrophotometry, SKB	SKB DL 0.006, RL 0.02	mg/L	25%
HS^-	Spectrophotometry, external laboratory	0.01	mg/L	0.02 (0.01–0.2 mg/L) 12% (> 0.2 mg/L)
NO_2 as N	Spectrophotometry	0.1	µg/L	2%
NO_3 as N	Spectrophotometry	0.2	µg/L	5%
NO_2+NO_3 as N	Spectrophotometry	0.2	µg/L	0.2 (0.2–20 µg/L) 2% (> 20 µg/L)
NH_4 as N	Spectrophotometry, SKB	11	µg/L	30% (11–20 µg/L) 25% (20–50 µg/L) 12% (50–1,200 µg/L)
NH_4 as N	Spectrophotometry external laboratory	0.8	µg/L	0.8 (0.8–20 µg/L) 5% (> 20 µg/L)
PO_4 as P	Spectrophotometry	0.7	µg/L	0.7 (0.7–20 µg/L) 3% (> 20 µg/L)
SiO_4	Spectrophotometry	1	µg/L	2.5% (> 100 µg/L)
O_2	Iodometric titration	0.2–20	mg/L	5%
Chlorophyll a, c pheopigment[7]	/1/	0.5	µg/L	5%
PON[7]	/1/	0.5	µg/L	5%
POP[7]	/1/	0.1	µg/L	5%
POC[7]	/1/	1	µg/L	4%
Tot-N[7]	/1/	10	µg/L	4%
Tot-P[7]	/1/	0.5	µg/L	6%
Al,	ICP SFMS	0.2, 0.3, 0.7[4]	µg/L	17.6%[6]
Zn	ICP SFMS	0.2, 0.8, 2[4]	µg/L	15.5, 17.7, 25.5%[6]
Ba, Cr, Mo,	ICP SFMS	0.01, 0.04, 0.1[4]	µg/L	Ba 15%[4], Cr 22%[5] Mo 39%[6]
Pb	ICP SFMS	0.01, 0.1, 0.3[4]	µg/L	15%[6]
Cd	ICP SFMS	0.002, 0.02, 0.5[4]	µg/L	15.5%[6]
Hg	ICP AFS	0.002	µg/L	10.7%[6]
Co	ICP SFMS	0.005, 0.02, 0.05[4]	µg/L	25.9%[6]
V	ICP SFMS	0.005, 0.03, 0.05[4]	µg/L	18.1%[6]
Cu	ICP SFMS	0.1, 0.2, 0.5[4]	µg/L	14.4%[6]
Ni	ICP SFMS	0.05, 0.2, 0.5[4]	µg/L	15.8%[6]
P	ICP SFMS	1, 5, 40[4]	µg/L	16.3%[6]
As	ICP SFMS	0.01 (520 mS/m)	µg/L	59.2%[6]
La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu	ICP SFMS	0.005, 0.02, 0.05[4]	µg/L	20%, 20%, 25%[6]
Sc, In, Th	ICP SFMS	0.05, 0.2, 0.5[4]	µg/L	25%[6]
Rb, Zr, Sb, Cs	ICP SFMS	0.025, 0.1, 0.25[4]	µg/L	15%, 20%, 20%[5] 25%[6]

Component	Method[1]	Reporting limits (RL), detection limits (DL) or range[2]	Unit	Measurement uncertainty[3]
Tl	ICP SFMS	0.025, 0.1, 0.25[4]	µg/L	14.3%[5 and 6]
Y, Hf	ICP SFMS	0.005, 0.02, 0.05[4]	µg/L	15%, 20%, 20%[5] 25%[6]
U	ICP SFMS	0.001, 0.005, 0.01[4]	µg/L	13.5%, 14.3%, 15.9%[5] 19.1%, 17.9%, 20.9%[6]
DOC	UV oxidation, IR Carbon analysator	0.5	mg/L	8%
TOC	UV oxidation, IR Carbon analysator	0.5	mg/L	10%
δ^{2}H	MS	2	‰ SMOW[8]	0.9 (one standard deviation)
δ^{18}O	MS	0.1	‰ SMOW[8]	0.1 (one standard deviation)
^{3}H	LSC	0.8	TU[9]	0.8
δ^{37}Cl	A (MS)	0.2	‰ SMOC[10]	0.2[17]
δ^{13}C	A (MS)	–	‰ PDB[11]	0.3[17]
^{14}C pmc	A (MS)	–	PMC[12]	0.4[17]
δ^{34} S	MS	0.2	‰ CDT[13]	0.4 (one standard deviation)
^{87}Sr/^{86}Sr	TIMS	–	No unit (ratio)[14]	0.00002
^{10}B/^{11}B	ICP SFMS	–	No unit (ratio)[14]	–
^{234}U, ^{235}U, ^{238}U, ^{232}Th, ^{230}Th	Alfa spectr.	0.0001	Bq/L[15]	≤ 5% (Counting statistics uncertainty)
^{222}Rn, ^{226}Ra	LSS	0.015	Bq/L	≤ 5% (Count. stat. uncert.)

1. Many elements may be determined by more than one ICP technique depending on concentration range. The most relevant technique and measurement uncertainty for the concentrations normally encountered in groundwater are presented. In cases where two techniques were frequently used, both are displayed.

2. Reporting limits (RL), generally 10×standard deviation, if nothing else is stated. Measured values below RL or DL are stored as negative values in Sicada (i.e. –RL value and –DL value).

3. Measurement uncertainty reported by the laboratory, generally as ± percent of measured value in question at 95% confidence interval.

4. Reporting limits at electrical cond. 520 mS/m, 1,440 mS/m and 3,810 mS/m respectively.

5. Measurement uncertainty at concentrations 100×RL.

6. Measurement uncertainty at concentrations 10×RL.

7. Determined only in surface waters. PON, POP and POC refers to Particulate Organic Nitrogen, Phosphorous and Carbon, respectively .

8. Per mille deviation[16] from SMOW (Standard Mean Oceanic Water).

9. TU = Tritium Units, where one TU corresponds to a tritium/hydrogen ratio of 10^{-18} (1 Bq/L Tritium = 8.45 TU).

10. Per mille deviation[16] from SMOC (Standard Mean Oceanic Chloride).

11. Per mille deviation[16] from PDB (the standard PeeDee Belemnite).

12. The following relation is valid between pmC (percent modern carbon) and Carbon-14 age:
$pmC = 100 \times e^{((1950-y-1.03t)/8274)}$
where y = the year of the C-14 measurement and t = C-14 age.

13. Per mille deviation[16] from CDT (the standard Canyon Diablo Troilite).

14. Isotope ratio without unit.

15. The following expressions are applicable to convert activity to concentration, for uranium-238 and thorium-232: 1 ppm U = 12.4 Bq/kg^{238}U, 1 ppm Th = 3.93 Bq/kg^{232}Th.

16. Isotopes are often reported as per mille deviation from a standard. The deviation is calculated as: $\delta yI = 1000\times(K_{sample}-K_{standard})/K_{standard}$, where K = the isotope ratio and ^{y}I = ^{2}H, ^{18}O, ^{37}Cl, ^{13}C or ^{34}S etc.

17. SKB estimation from duplicate analyses by the contracted laboratory.

3 Reliability of drilling water contents

The determination of drilling water contents in water samples was based on analyses of the dye uranine which was used to trace the drilling water (nominal concentration 0.2 mg/L) during drilling of the cored boreholes. Samples for uranine analyses were collected at different occasions and for the following purposes:

1. To check the stability of the automatic dosing of uranine to the drilling water used during drilling and to determine the drilling water content in the return water in order to calculate a drilling water budget from drilling the borehole, see Table 3-1.
2. To monitor changes in the drilling water content during borehole clean up pumping and nitrogen flushing (N_2 class 2 quality) conducted in order to decrease the drilling water content in the boreholes prior to hydrogeochemical investigations.
3. To determine the drilling water content in the water samples collected during the subsequent hydrogeochemical investigations. The drilling water content in each borehole sample was calculated from the average uranine concentration in the drilling water when drilling the borehole. No corrections were made for variations in the uranine dosing to the drilling water.

The fluorescence method used to determine the uranine concentration is straightforward and quite reliable down to about 0.3 μg/L, corresponding to 0.15% drilling water. However, factors other than analytical errors may obstruct the different interpretations.

Additional fluorescence from organic constituents in the groundwater has been reported as a source of errors. Two tests /Nilsson 2008/ were conducted in order to check the effect of groundwater organics on the measured uranine concentration:

- Fluorescence measurements in several blanks consisting of near-surface groundwater samples from Forsmark site investigation with varying and high contents of TOC (Total Organic Carbon) see Table 3-2.
- Uranine was added at a concentration of 10 μg/L to different Forsmark waters with TOC concentrations in the range usually encountered in the sampled groundwaters. The fluorescence was measured before and after the additions and the corresponding uranine concentrations were recorded, see Table 3-3. The observed interference from TOC was not linear which may be due to different character of the organic constituents.

From the tests it was concluded that the effect from TOC is relatively small and most often negligible. Factors that are more likely to interfere with drilling water interpretations are:

- Unstable/inhomogeneous uranine concentration in drilling water injected into the borehole. Generally, the uranine concentration differed within ± 10% but problems with the dosing occurred at times for a few boreholes. The average uranine concentrations and standard deviations in the drilling water samples collected during drilling are given for each borehole in Table 3-1.
- Inadequate mixing prior to sampling of drilling water for uranine analyses and therefore inhomogeneous uranine concentration. The uranine concentration in the drilling water injected into the borehole will seem to vary more than is really the case.
- Too few samples or bias in the sampling (i.e. all samples collected at the same drilling situation – for example just after core retrieval) may result in unrepresentative average uranine concentrations for the drilling water injected into the borehole and for the return water withdrawn from the borehole. Sampling of return water with a highly varying content of drilling water is especially critical in order to obtain a consistent drilling water budget.

An attempt to calculate/estimate the amounts of uranine added and withdrawn from each borehole and make a rough estimate of the remaining volume of drilling water is presented in Table 3-1. Lack of information on the weighed total amount of uranine added to each borehole, together with uncertain flow/volume measurements for some boreholes (especially boreholes KLX13A and KLX27A) obstructs the estimations. A comparison between weighed "true" and calculated added amount of uranine, made from Forsmark data /Nilsson 2008/, revealed relatively large uncertainties in the calculated values probably due to not representative enough average uranine concentrations. This is probably the case also in Laxemar. Therefore the volume information in the table should be considered as merely indicative.

Table 3-1. Uranine additions to drilling water, uranine recovery from return water and drilling water budget from core drilling.

Borehole ID code	Average* uranine conc. and standard deviation; drilling water (mg/L)	Estimated amount of uranine in drilling water** (g)	Average* uranine conc. and standard deviation; return water (mg/L)	Estimated amount of uranine recovered in return water** (g)	Estimated volume of drilling water remaining in the borehole after drilling (m³)
KLX08A	0.188 ± 0.042	187 (119)	0.019 ± 0.026	47 (125)	700
KLX13A	0.219 ± 0.021	171 (107)	0.070 ± 0.054	175 (107)	0
KLX15A	0.196 ± 0.020	207 (133)	0.113 ± 0.036	193 (133)	70
KLX17A	0.218 ± 0.019	137 (87)	0.146 ± 0.040	157 (87)	0
KLX27A	0.230 ± 0.035	130 (89)	0.136 ± 0.061	261 (89)	0

* Average and std. as calculated from the number of samples given within parentheses in next column.
** The amount of uranine is calculated using total volumes of drilling water and return water together with the average uranine concentrations from the number of samples given within parentheses.

Table 3-2. Fluorescence measurements – analyses of near surface groundwater samples with uranine concentration = zero at high and varying TOC concentrations (Total Organic Carbon).

Idcode (Forsmark boreholes)	Water type	TOC (mg/L)	Corresponding uranine concentration (µg/L) from blank fluorescence
SFM0087	Near surface groundwater	19.7	0.7
SFM0095	Near surface groundwater	20.0	1.2
SFM0032	Near surface groundwater	20.9	1.0
SFM0037	Near surface groundwater	22.9	1.3
SFM0049	Near surface groundwater	23.3	0.7
SFM0001	Near surface groundwater	24.6	1.0
SFM0102	Near surface groundwater	125	3.5

Table 3-3. Analyses of uranine standard solutions (10 µg/L) prepared from waters with different TOC concentrations.

Idcode (Forsmark boreholes)	Water type	TOC (mg/L)	Corresponding uranine (µg/L) from blank fluorescence	Recovery, 10 µg/L uranine
–	Deionised water	0–0.5	0 (adjusted to zero)	9.9
HFM27	Groundwater	5	0.7	9.7
HFM01	Groundwater	10	0.6	10.9
HFM16	Groundwater	13	1.0	10.6
PFM000074	Lake water	20	0.3	9.8

4 Quality of basic water analyses

Major constituents

In order to establish a consistent set of major constituent concentrations (mainly Na, Ca, Cl , SO_4 and possibly Mg and HCO_3) for each sample, the first step was to compare chloride concentrations and electrical conductivity values in x-y diagrams. The diagram in Figure 4-1 includes chloride concentrations and EC values (field-EC or lab-EC) as reported in SKB database Simon. The diagram shows that the main part of the 2,470 data points follow the trend line and indicate that the EC and chloride data sets are internally consistent.

The relative charge balance gives an indication of the quality and uncertainty of the analyses of the major ions and, together with the chloride – EC correlation; they were used to verify that the concentrations of the most dominant ions were consistent. The errors, as calculated for the samples in SKB database Simon, seldom exceeded the acceptable limit ± 5% (14 samples) and ± 10% (16 samples) for groundwater and dilute surface waters, respectively. These limits are set in the QA system in advance.

ICP AES analyses

Several major ions were determined by ICP-AES (Inductively Coupled Plasma Atomic Emission Spectrometry). All samples were analysed by a regular laboratory (lab 1) and replicate analyses were conducted for a minor part of the samples (99 samples) by a second checking laboratory (lab 2). The agreement between the reported concentrations from the two laboratories was not always satisfactory, see Figures 4-2a to f. Despite this, the selected concentrations (almost exclusively lab 1) were regarded as fully reliable and of good quality based on high stability of concentrations in time series, small charge balance errors (dominant ions) and check by other analytical methods (iron, sulphate, bromide, uranium). The checking laboratory (lab 2) was less familiar with the type of saline groundwater samples being analysed. In the cases of iron and sulphur analyses, see below, the results from lab 1 showed better agreement with the second method than the results from lab 2.

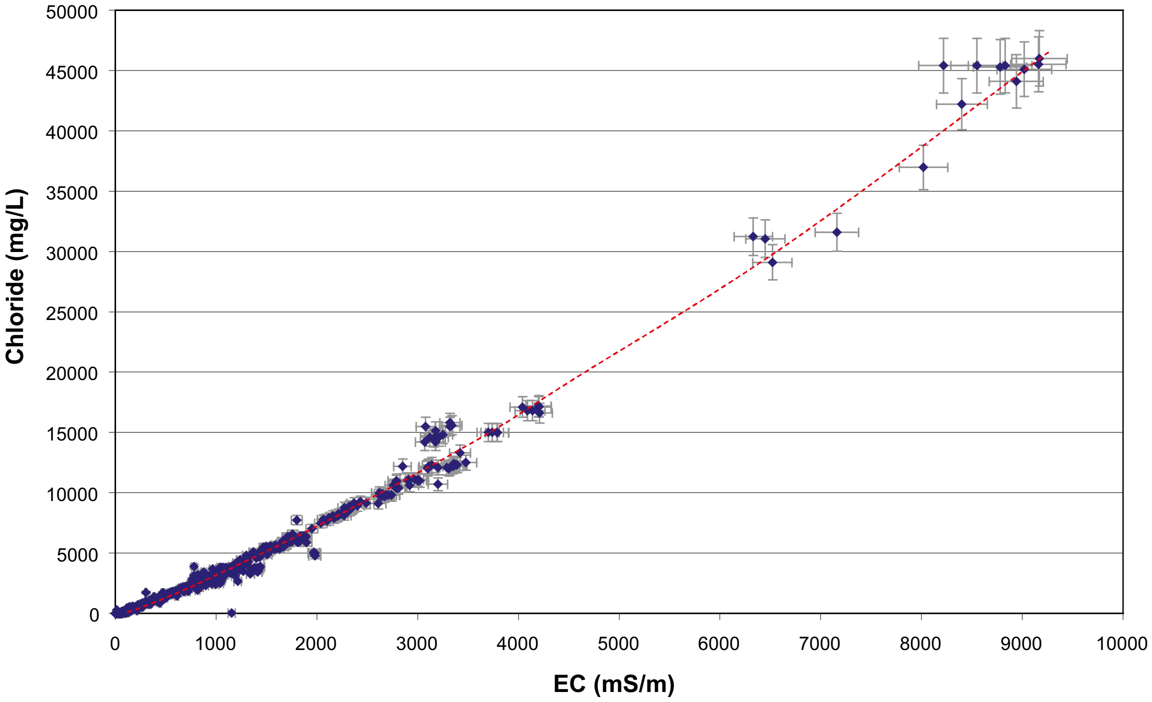


Figure 4-1. Chloride concentrations plotted versus EC values (SKB database Simon).

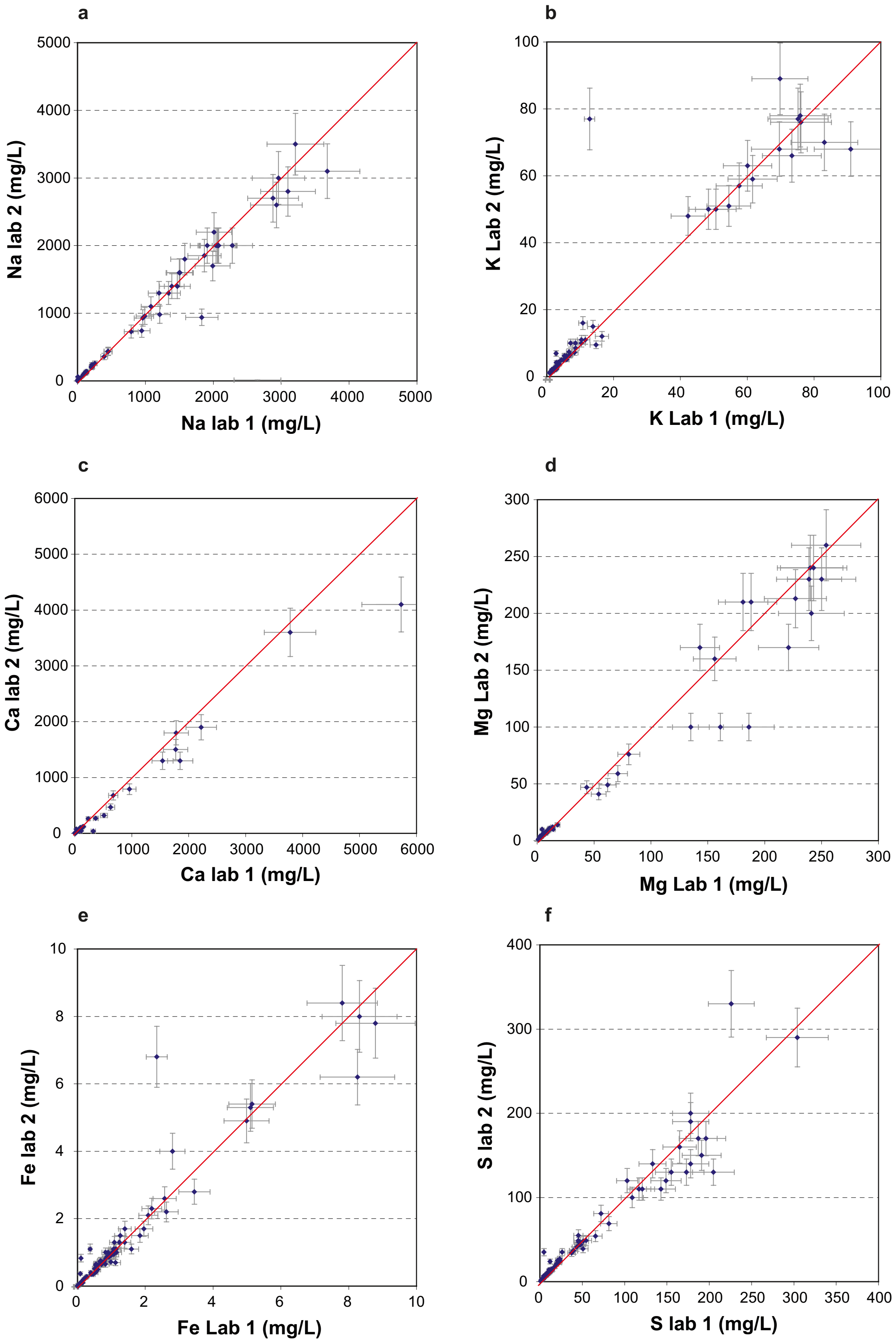


Figure 4-2a to f. *Comparison of Na, K, Ca, Mg, Fe and S concentrations by ICP AES reported by the regular laboratory (lab 1) and the checking laboratory (lab 2). 99 duplicate analyses.*

Sulphate

Sulphate and elemental sulphur were determined regularly in every sample by Ion Chromatography (IC) and ICP-AES, respectively, see Figure 4-3. Generally, the agreement between the IC and the ICP-AES results by the two regular laboratories was satisfactory.

The ICP-AES analyses of sulphur may be affected by the presence of sulphide at high concentrations. If hydrogen sulphide gas from the acidic sample enters the plasma it causes a disproportionate increase in sulphur.

Bromide

At high chloride concentrations, the bromide analyses obtained by IC may be affected by a contribution from the chloride peak, resulting in too high concentration values. Another drawback with the method is the relatively high detection limit (0.2 mg/L). The bromide concentrations in many surface waters measured below or close to the detection limit. For these reasons, complementary analyses of bromine by the ICP-SFMS technique were performed rather frequently in order to check and verify the bromide results. Some obviously erroneous results have been reported also from the ICP-SFMS method.

A comparison of the analytical results by IC and by ICP-SFMS is presented in Figure 4-4. As demonstrated, the spread is not alarming. Selected bromide values (often the ICP-SFMS results) for each sample are plotted versus the corresponding chloride concentrations in Figure 4-5 as a rough consistency check. The data points form two relatively clear trends (mixing lines). The two different trends correspond to marine and non-marine origin, respectively, and values between the lines may be a result of mixing of the two water types. The bromide analyses, whatever analytical method used, were impaired by larger uncertainty than most other major constituents. However, the frequent possibility to compare results from two different methods and the careful selection of data improved the final bromide data set. Generally, if values from

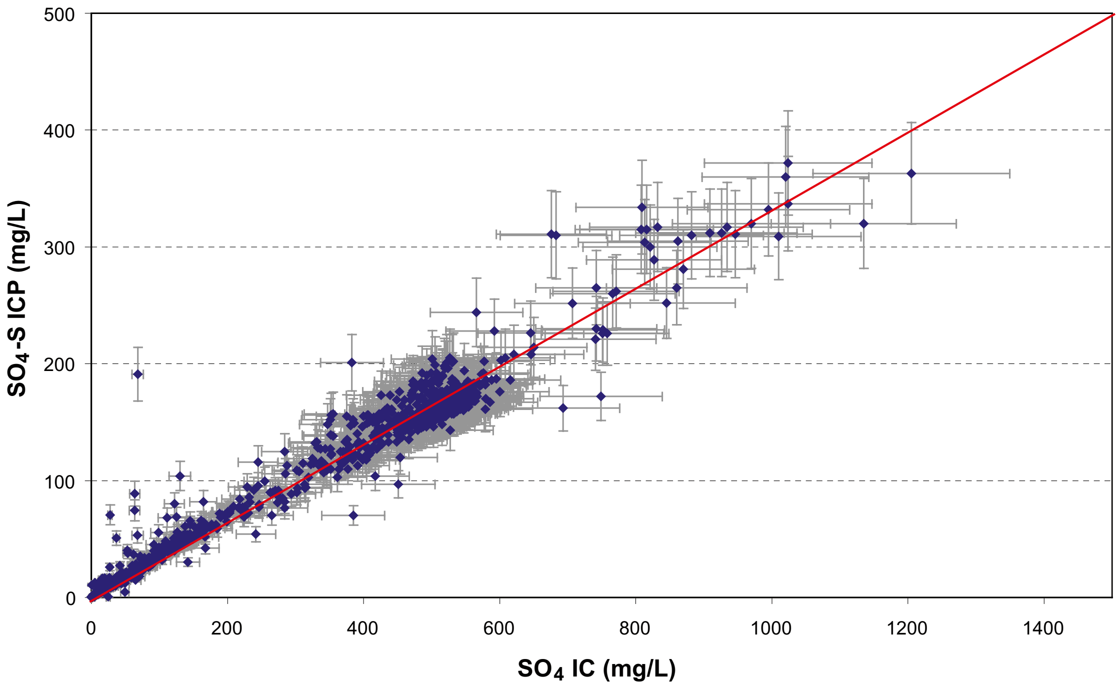


Figure 4-3. *Comparison of sulphur by the ICP-AES technique (lab 1) and sulphate by IC. Without significant contribution of other sulphur species, 3×*SO_4*-S by ICP should correspond to* SO_4 *by IC.*

both methods were available and they agreed within 15%, IC values were selected. If the two methods disagreed or if only IC results were available, a judgement of plausibility was made. This was based on comparison with other samples from the same object, evaluation of water type and bromide versus chloride plots. Marine waters often show bromide/chloride ratios of approximately 0.0035 whereas ratios around 0.01 are more typical of water/rock interaction.

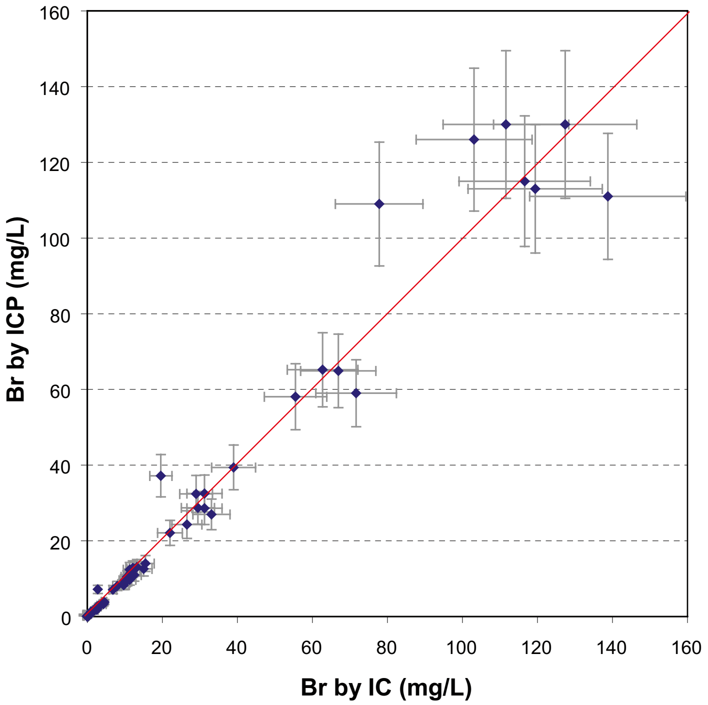


Figure 4-4. *Comparison of bromine by ICP technique (lab 1) and bromide by IC, 56 samples. The error bars correspond to 15% (IC and ICP).*

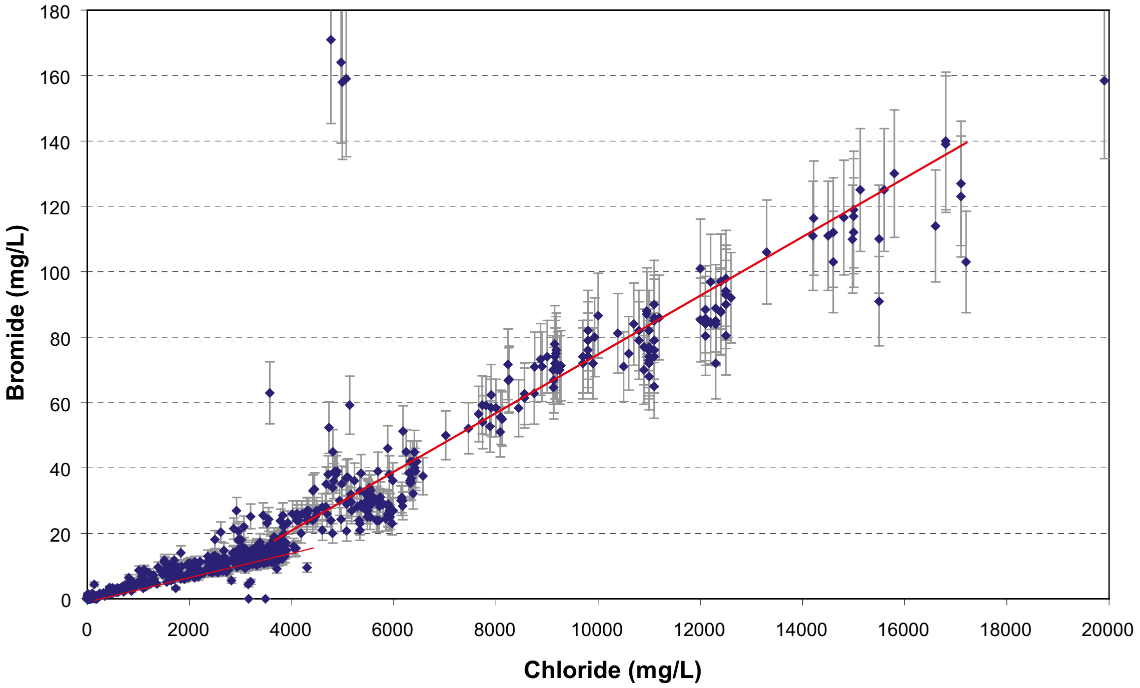


Figure 4-5. *Bromide values as selected in SKB database Simon plotted versus chloride concentrations (samples with Cl < 20,000 mg/L). The error bars correspond to ± 15%. Assumed mixing trends are indicated as lines.*

Iron

The risk of impacting the iron concentration from pumping flow rate changes and/or processes such as sorption/ desorption on/from long tubing, filters or other equipment can not be disregarded for deep groundwaters. However, comparisons between iron concentrations by ICP AES and by the spectrophotometric method indicated if short time variations occurred. Furthermore, reproducible and repeatable results from different sampling methods and/or sampling occasions strengthen the credibility of both the methodology and data.

Total/ferrous iron and elemental iron were determined regularly by a spectrophotometric method and by ICP-AES, see Figure 4-6. The ICP analyses often resulted in higher concentrations than the spectrophotometric method. This is probably due to the presence of a colloidal phase. The spectrophotometric method does not include, or only partly includes, possibly bound iron that passes a 0.40 μm filter, but the ICP method makes no distinction between different iron containing species.

Sulphide

Sulphide was determined by a spectrophotometric method and at only one laboratory. The results for some tens of Forsmark samples /Nilsson 2008/ with duplicate analyses by two laboratories showed satisfactory agreement and there is no obvious reason why the quality should be different for samples from Laxemar. The reliability is also confirmed by the generally very stable hydrogen sulphide concentrations obtained within sample series collected during pumping and sampling periods. However, late samples from the monitoring programme indicate increased and varying concentrations that seem to relate to the pumped volume from the borehole section.

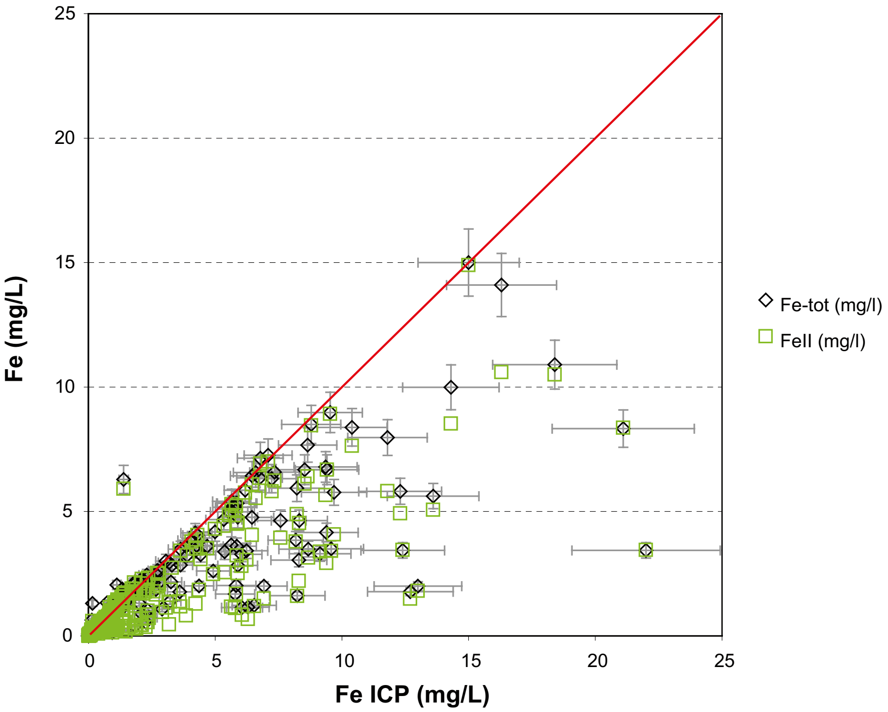


Figure 4-6. *Comparison of iron concentrations. Total and ferrous iron by a spectrometric method are plotted versus elemental iron determined by ICP-AES at the regular laboratory (lab 1).*

5 Quality of isotopic analyses

Uranium-238 activity and uranium concentration

In total, 170 samples of surface and groundwaters were analysed for both uranium concentration by ICP MS and for uranium-238 by alpha spectroscopy. The two different uranium determinations are compared in Figures 5-1a and 5-1b. The initial laboratory for U-238 determinations was changed due to unacceptably high detection limit (50 mBq/kg corresponding to 4.03 µg/L). A few samples have activity results only from this first laboratory (lab a) and as shown in the diagram the agreement is less satisfactory for those samples. Generally, the determinations of uranium element concentrations and uranium-238 activities show reasonable agreement considering the different analytical techniques and the often very low concentrations.

Deuterium, oxygen-18 and carbon isotopes

The results of duplicate analyses of deuterium, oxygen-18 and carbon isotopes by two independent laboratories on a limited number of samples from Forsmark /Nilsson 2008/ illustrate the reliability of the determinations also for Laxemar samples. The isotope results from the regular laboratory (lab 1) and the checking laboratory (lab 2), are compared in Figures 5-2 to 5-5. Generally, the agreement between the laboratories was satisfactory, but some discrepancies exist (e.g. $\delta^{13}C$). The average standard deviations for deuterium and oxygen-18 were similar to the reported measurement uncertainties from the contracted laboratories and amounted to 1.1‰ SMOW and 0.2‰ SMOW, respectively.

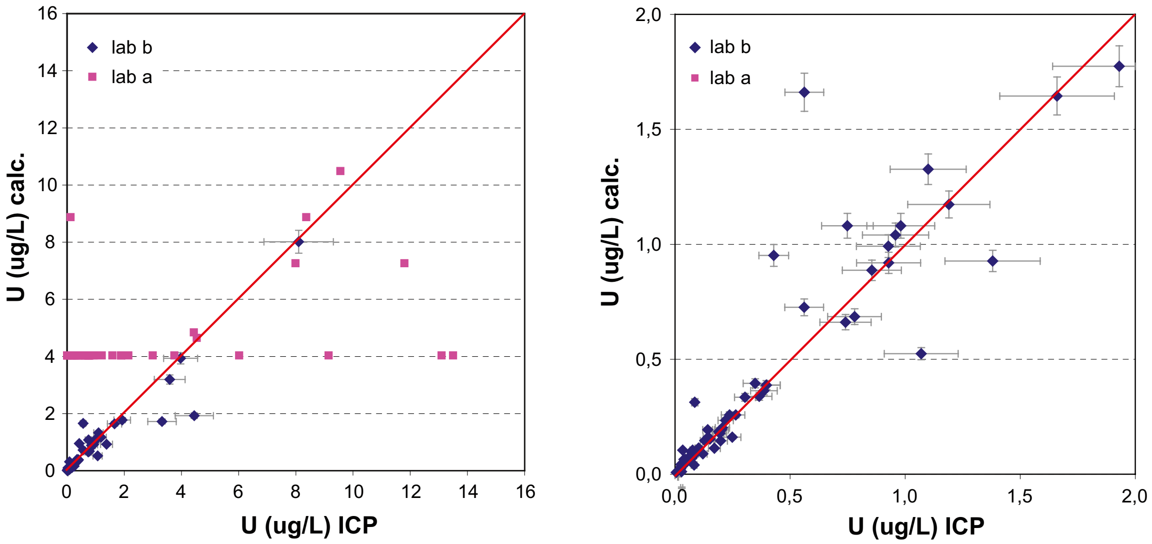


Figure 5-1. ***a.*** *Comparison of uranium concentrations (µg/L) by ICP-MS and calculated from uranium-238 activities for a total of 170 samples. 1 ppm U = 12.4 Bq/kg* ^{238}*U.* ***b.*** *Limited concentration range 0-2 µg/L.*

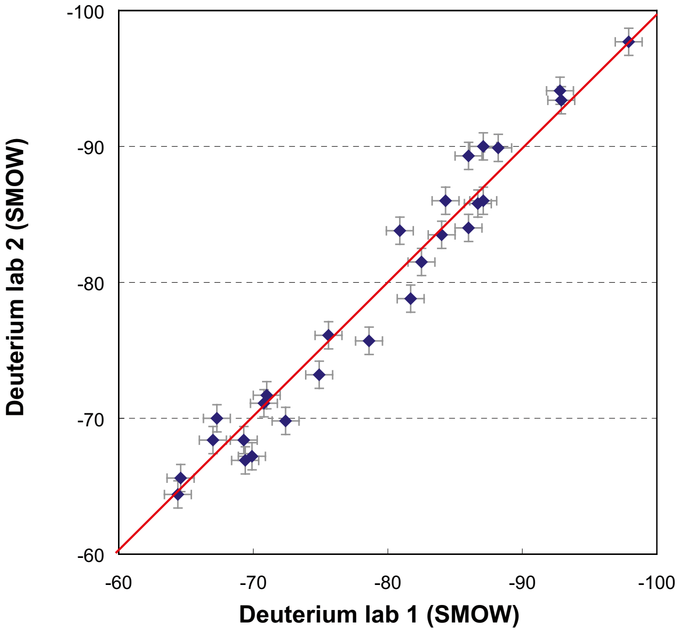


Figure 5-2. *Comparison of duplicate deuterium analyses. Deuterium (δ²H‰ SMOW) was determined by a regular laboratory (lab 1) and a checking laboratory (lab 2) for 27 samples from Forsmark.*

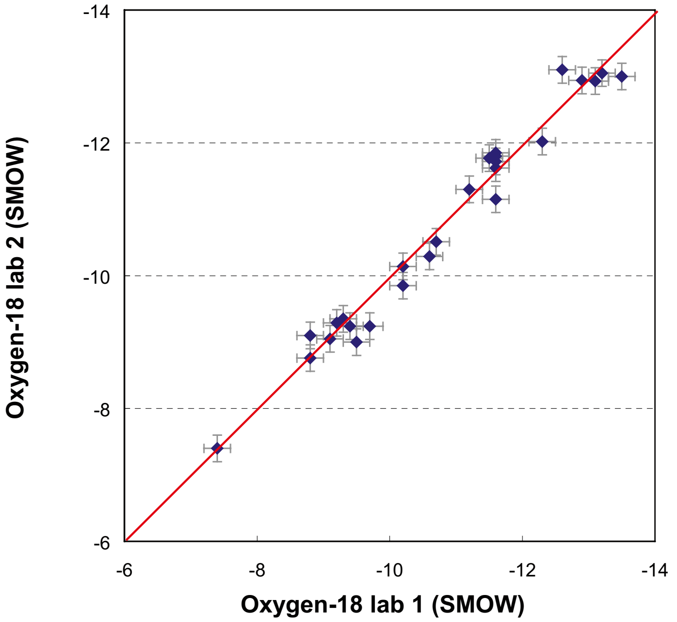


Figure 5-3. *Comparison of duplicate oxygen-18 analyses. Oxygen-18 (δ¹⁸O‰ SMOW) was determined by a regular laboratory (lab 1) and a checking laboratory (lab 2) for 27 samples from Forsmark.*

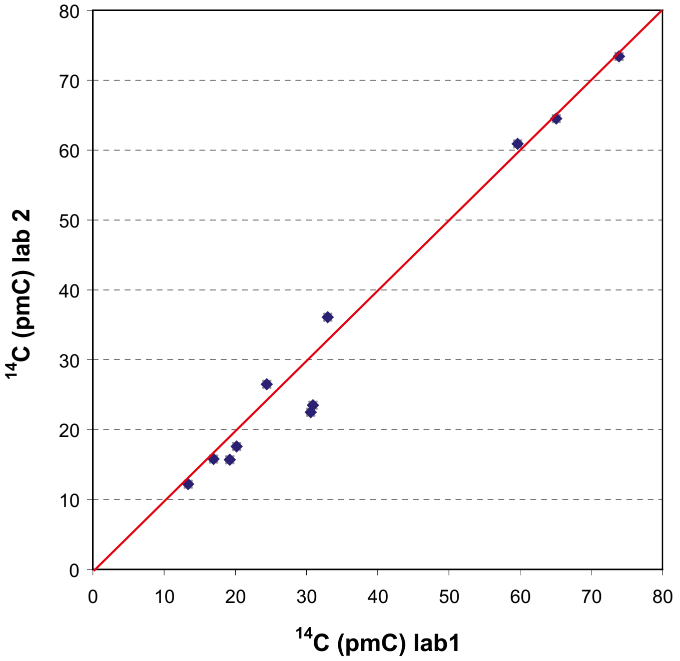


Figure 5-4. *Comparison of duplicate pmC determinations. Determinations of pmC (TIC) were performed by a regular laboratory (lab 1) and a checking laboratory (lab 2) for 11 samples from Forsmark.*

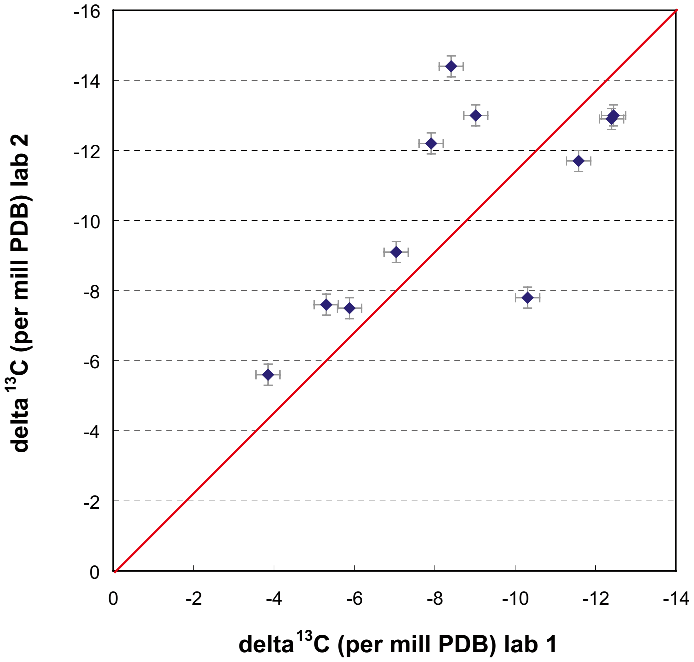


Figure 5-5. *Comparison of duplicate δ^{13}C determinations. δ^{13}C was determined by a regular laboratory (lab 1) and a checking laboratory (lab 2) for11 samples from Forsmark.*

6 Conclusions

- Factors such as unstable additions or inhomogeneous mixing of the uranine dye to the drilling water used for drilling caused errors in the determination of drilling water contents. The impact from these shortcomings in the large scale drilling water treatment in the field was most probably larger than from the errors in the analyses of the uranine. The stability of the uranine concentration in the drilling water injected into each core drilled borehole is an indication to the reliability of the drilling water determinations. From Forsmark data it was found that errors caused by additional fluorescence from TOC were relatively small and negligible and it is assumed also to be the case here.
- The reported general measurement uncertainties from the contracted laboratories often seem to be somewhat large when compared to the impression from trend plots and other consistency checks. Especially, the measurement uncertainties for the analyses of major ions seem to be overestimated. Nevertheless, the values are accepted for the moment because individual datum point uncertainties cannot yet be integrated into the Sicada database system.
- There is high confidence in the set of major constituents for each sample. Independent methods and/or duplicate analyses were used to check the consistency of the major ions and to confirm the concentrations of chloride, sulphate, bromide and iron.
- The bromide analyses were found to be somewhat more uncertain than most other major ions. However, the frequent use of two different methods (IC and ICP-SFMS), comparison of the two results and check of Br/Cl ratios, improved the final bromide data set.
- Two commercial laboratories conducted ICP-AES and ICP-MS analyses. All samples were analysed by the regular laboratory (long cooperation with SKB and with universities) and duplicate analyses were carried out for a minor part of the samples by a checking laboratory (general routine laboratory). The performance of the two laboratories was not comparable and results from the regular laboratory were reported almost exclusively.
- Apart from analytical errors and contamination problems, the analytical results may be biased by sampling equipment, sampling methods or sampling conditions. Factors such as sorption on long tubing or effects from varying pumping flow rates may affect, for example, the concentrations of iron and other trace metals and probably also microbial activity and indirectly the hydrogen sulphide concentrations. The reproducibility and stability of the water compositions on different occasions and conditions indicated if this was a problem or not.
- Duplicate isotope determinations from Forsmark samples showed good agreement and verify the quality of carbon isotopes, oxygen-18 and deuterium determinations also from Laxemar. The uranium-238 data by alpha spectroscopy and the uranium element concentration by ICP-SFMS were generally consistent.

7 References

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Section 5

Determination of residence time based on ^{4}He and ^{36}Cl of Laxemar groundwaters

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Contents

1 Introduction

Several methods exist for determining the residence time[1] of groundwaters in fractured rocks. These include determining rates of solute or gas accumulation, identifying species characteristic of climatic conditions, and using the rates of decay (or ingrowth) of radioactive elements. Groundwaters have been extensively sampled from permeable fractures and fault zones in boreholes up to 1.6 km deep at Laxemar, Sweden, as part of the site characterisation studies for the Swedish nuclear fuel waste disposal program.

Five end-member water types have been identified at the Laxemar site /Gurban 2008, section # 1, this report/:

- **Deep Saline end-member:** Brine type of reference water**,** represents the deep brine type (Cl = 47,000 mg/l) of water sampled from borehole KLX02: 1,631–1,681 m /Laaksoharju et al. 1995/. An old age for the Deep Saline is suggested by the measured ^{36}Cl values indicating a minimum residence time of 1.5 Ma for the Cl component /Laaksoharju and Wallin 1997/.
- **Glacial end-member:** Represents a possible melt-water composition from the last deglaciation > 12,000 BC. Modern glacial melt water from Norway was used for the major elements and the δ^{18}O isotope value (−21‰ SMOW) was based on measured values of δ^{18}O in calcite surface deposits /Tullborg and Larson 1984/. The δ^{2}H value (−158‰ SMOW) is a modelled value based on the global relationship ($\delta^2H = 8 \times \delta^{18}O + 10$) for the meteoric water line.
- **Old Meteoric-Glacial end-member:** In order to better predict the δ^{18}O values, a mixture of Old Meteoric-Glacial type of water was used as an end-member. This water has δ^{2}H = –118‰ and δ^{18}O = –16‰.
- **Littorina Water end-member:** Represents modelled Littorina water. The Littorina composition is more saline than the current Baltic sea composition. Therefore Littorina water is used in the calculations.
- **Altered meteoric end-member:** Corresponds to an upper bedrock water composition, obtained by the infiltration of meteoric water (the origin can be rain or snow) in the bedrock.

Evidence for the intrusion of Littorina seawater at Laxemar is mainly based on the fact that certain groundwaters from an intermediate depth range (typically 300–500 m have significantly higher Mg and SO_4 and lower HCO_3 concentrations than overlying fresh groundwaters and the underlying glacial waters. /Pitkänen et al. 1996/ have argued that these waters probably infiltrated during the Littorina Sea stage when much of the shield rocks in this area were still below sea level.

Helium-4 and ^{36}Cl are useful isotopic tracers for determining the residence time of groundwater or for identifying mixing of groundwaters and the characteristics of water-rock interaction. This report describes the results of ^{4}He and ^{36}Cl analyses of selected groundwater types at the Laxemar-Simpevarp area to determine if the data support the proposed Littorina origin of this high Mg–SO_4 type of groundwater. Comparison is made with results from other sites.

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[1] Groundwater residence time is sometimes confused with the 'age' of a groundwater. As pointed out by /Clark and Fritz 1997/, "Only tritium is part of the water molecule and can actually 'date' the water. All other dating methods rely on dissolved constituents whose abundance in water is controlled by physiochemical and biological processes. Groundwater mixing inevitably averages out the age, especially in fractured rock, and various 'dating' methods should be used to derive an average residence time".

2 Groundwater residence time: Theory

2.1 Helium-4

Helium-4 is continuously being produced in rocks as alpha particles emitted in the decay of the naturally occurring radioactive elements, uranium and thorium, and their radioactive daughters. Helium-4 is the most abundant of the He isotopes ($^3He/^4He = 1.38\times10^{-6}$, /Andrews et al. 1989a, b/) and so ^4He is usually abbreviated to He. Helium-3, while having characteristic concentrations in the various reservoirs of the earth, is rapidly diluted by ^4He produced in the geosphere and so has no characteristic value in the upper crust.

Helium is both conservative and chemically inert but, unlike Cl in groundwater, its concentration in the atmosphere is very low (5.24 ppm) and the amount of He recharged via precipitation (48 μcm^3/L water) is insignificant compared to the He produced in situ /Solomon 2000/. Radiogenic He produced in U- and Th-bearing minerals in the bedrock can be slowly released to adjacent porewater by dispersion and then migrate out into fractures and transported to the surface either through soil gases or at groundwater discharge sites /Gascoyne and Sheppard 1993/. Information on groundwater residence time and mixing with other He sources can be obtained by comparing measured He concentrations in groundwater with those calculated from in situ He-production rate.

The decay of each atom of the parent radionuclides ^{238}U, ^{235}U and ^{232}Th, to their respective Pb isotopes, produces a total of 8, 7 and 6 alpha particles, respectively. In a state of slow-moving or stagnant groundwater, the rate of He production may attain steady state with the loss of He by diffusion through groundwater out of the site. In this case, the rate of He release into the groundwater (G) is given by /Pearson et al. 1991/:

$$G = \rho\, N_L\, \{8\, [^{238}U]\, (\lambda_{238}/M_{238}) + 7\, [^{235}U]\, (\lambda_{235}/M_{235}) + 6\, [^{232}Th]\, (\lambda_{232}/M_{232})\} \qquad \text{Equation 2-1}$$

where:

G is the ^4He release rate per unit volume of solids per unit time (atoms $m^{-3}\ s^{-1}$),
ρ is the density of solids ($g\ m^{-3}$),
N_L is Avogadro's Number (6.022×10^{23} atoms mol^{-1}),
λ_{238}, λ_{235} and λ_{232} are the decay constants for ^{238}U, ^{235}U and ^{232}Th ($4.92\times10^{-18}\ s^{-1}$, $3.12\times10^{-17}\ s^{-1}$ and $1.57\times10^{-18}\ s^{-1}$, respectively),
M_{238}, M_{235} and M_{232} are their respective molecular weights ($g\ mol^{-1}$), and
$[^{238}U]$, $[^{235}U]$ and $[^{232}Th]$ are the decimal fractions of ^{238}U, ^{235}U and ^{232}Th in solids ($g\ g^{-1}$).

Typical ^{238}U, ^{235}U and ^{232}Th concentrations in igneous and sedimentary rocks are 5×10^{-7} to 4×10^{-6}, 5×10^{-9} to 4×10^{-7}, and 1.5×10^{-6} to 1.5×10^{-5} $g\ g^{-1}$, respectively.

These values give ^4He release rates ranging from 0.28 to 2.4 μcm^3 (STP) $m^{-3}\ yr^{-1}$.

When the only source of ^4He is as described above, the groundwater age (τ) is given by

$$\tau = C_w/\{GC_1[(1/n) - 1]\} \qquad \text{Equation 2-2}$$

where C_w is the concentration of radiogenic ^4He (μcm^3 STP m^{-3}), n is the fractional porosity and C_1 is a conversion factor (3.7197×10^{-14} μcm^3 STP $atom^{-1}$).

In our calculations we used the following values:

$\rho = 2.7$ ($g\ cm^{-3}$),
$n = 0.25\%$
^{238}U, ^{235}U and ^{232}Th concentrations: average values of the above ranges, respectively: 2×10^{-6}, 2×10^{-7}, and 7×10^{-6} $g\ g^{-1}$ resulting in $G = 1.5$ μcm^3 (STP) $m^{-3}\ yr^{-1}$.

Using these values in the above formula the groundwater ages were calculated for the Laxemar subarea (Laxemar), Simpevarp peninsula (Simpevarp) Åspö island (Äspö) and Forsmark.

In Figure 2-1, the He-concentrations measured in the Forsmark and Laxemar-Simpevarp-Äspö groundwaters are plotted against the calculated groundwater ages. Linearity is expected because calculated ages are determined from measured He concentrations while all other parameters are held constant. However, the calculations show that the calculated ages are very high. They are in agreement with those obtained by /Smellie et al. 2008/, but show the limitations of the calculation method. For example, to obtain the measured He concentrations in the brackish marine (Littorina) groundwaters would have required about 50,000–100,000 to produce the equivalent He concentration in situ by radioactive decay. Even if these Littorina-type groundwaters contain a certain percentage of a very old component, these calculated time intervals are unrealistically long and, in turn, are assumed to indicate that there is an additional, substantial helium flux from greater depth

The high apparent ages determined from He-age calculations (when compared with other methods, e.g. ^{14}C) are a common characteristic in fractured rock and can, instead, be explained by release of old He during low-temperature alteration (weathering) of fractured rock in the upper flow systems of a crystalline rock formation. The He released in this situation has no bearing on the age of the groundwater in which it is dissolved because this He was formed and entrained at a much earlier time, quite possibly before the fracture was formed. Only now is it being released due to dissolution or alteration of the rock minerals.

2.2 Chlorine-36

Chlorine-36 is produced in rocks mainly by neutron capture by ^{35}Cl (which makes up about 75% of total Cl). The thermal neutrons for this reaction are produced during spontaneous fission of ^{238}U and by interactions between α particles (from decay of U and Th) and light elements such as Al, Na, O, Mg and Si in surrounding rocks /Florkowski et al. 1988/.

Unlike He, ^{36}Cl is radioactive and has a half-life of 301,000 years. It behaves conservatively, in exactly the same manner as stable Cl and is useful for identifying possible origins of dissolved stable Cl in ancient saline groundwaters extending back to early Quaternary and late Tertiary times /Andrews et al. 1989a, b, Bentley et al. 1986, Andrews and Fontes 1992, Clark and Fritz 1997/.

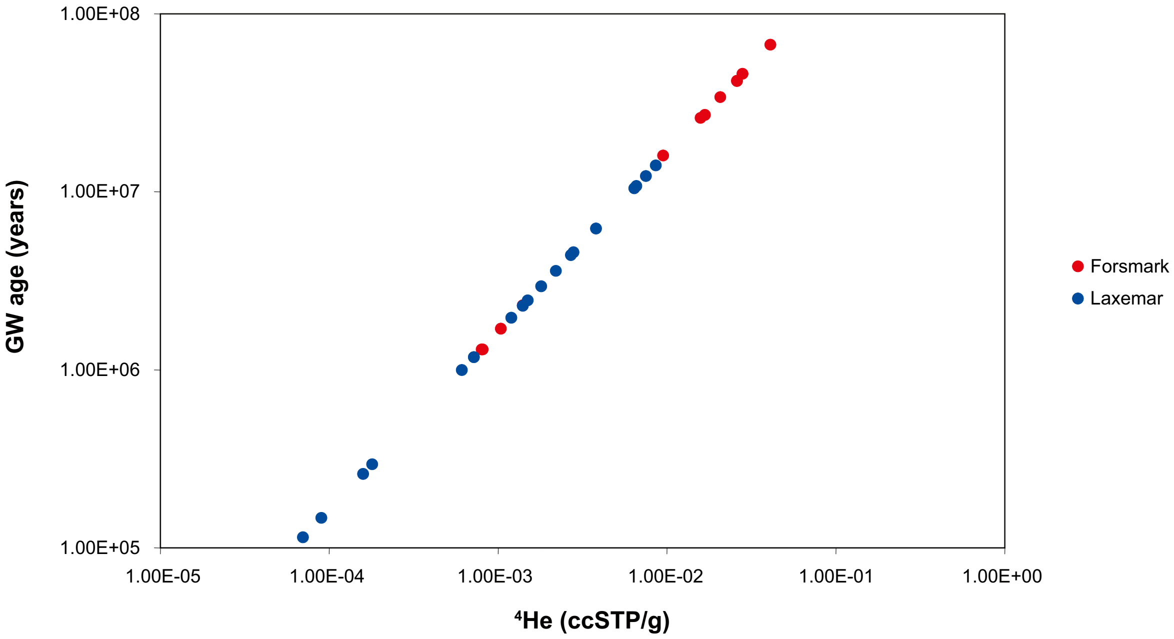


***Figure 2-1.** Calculated groundwater ages versus measured helium concentrations in groundwater at Forsmark and Laxemar (model ages neglect flux from great depth).*

Chlorine-36 in groundwaters has three sources: a) cosmic radiation in the upper atmosphere and rain-out, b) spallation of Cl, K, Ca, and Ar in soil moisture and minerals and c) subsurface production by neutron activation of stable ^{35}Cl from decay of naturally occurring radioelements (i.e. U, Th) at greater depth in the bedrock ^{36} Cl. With time, the ^{36} Cl will accumulate and decay until the rate of production equals the rate of decay (i.e. secular equilibrium) after a period of 1.5 million years. Groundwaters with ^{36}Cl values at secular equilibrium with in situ ^{36}Cl will therefore have been shielded from the atmosphere and resided in this rock for at least 1.5 million years.

Chlorine-36 has been measured in selected groundwaters from the Forsmark and Laxemar sites, ranging from the present Baltic Sea to near-surface recharge groundwaters, to deeper brackish marine (Littorina) and brackish non-marine groundwaters, and finally to saline groundwaters sampled from maximum depths.

To calculate the in situ ^{36}Cl production rate at a site and, hence, the equilibrium ^{36}Cl/Cl ratio of the associated groundwaters, the neutron production rate and initial neutron energy spectrum must be estimated from the U and Th contents of the rock (J. Fabryka-Martin, pers. comm.). The neutron flux and, consequently, the production rate of ^{36}Cl, is then calculated using a Monte Carlo neutron transport code for the average elemental composition of the rock types at the site. Rock compositional data, rock porosity, bulk density and rare earth concentrations (particularly gadolinium (Gd) and samarium (Sm)), are essential parameters in the calculation of neutron production rate and flux. Gadolinium is important because it has a very large thermal neutron cross-section and is able to stop all or much of the neutron flux despite its normally low (ppm) concentration in crystalline rocks.

The calculation of ^{36}Cl concentration is a complex undertaking, requiring proprietary codes and is not always possible to complete because of the lack of data. Calculations were made several years ago for the Olkiluoto site by J. Fabryka-Martin of the Los Alamos National Laboratory, New Mexico, and were reported by /Gascoyne 2001/.

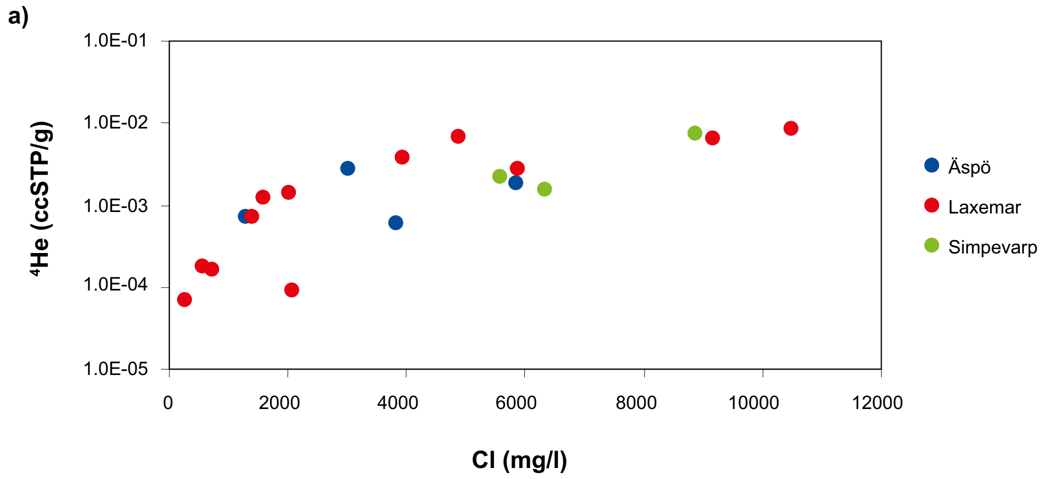
3 Results

As described above, the ^{4}He and ^{36}Cl contents of groundwaters can be used to give estimates of the residence time of groundwaters in the subsurface environment at Laxemar-Simpevarp-Äspö and, subsequently, compared with other Baltic sites.

3.1 Helium-4

Figure 3-1 shows the relationship between measured He and depth/Cl for Simpevarp/Laxemar/Äspö groundwaters. It can be seen that all groundwaters contain between 0.1 and 10 mL/L He and there is a general trend, particularly in the Laxemar data, to higher He concentrations with increasing depth. The low He values at shallower depths may be due to the presence of highly transmissive zones whereas the gradual He trend with depth likely reflects increased residence time and/or rock-water interaction.

A further indication of the age relationships of the Forsmark and Laxemar-Simpevarp-Äspö He data is seen in the comparison of He with δ^{18}O shown in Figure 3-2, Here, the lower trend suggests mixing of low-He groundwaters with cold-climate water but as He concentration increases, the upper trend indicates increasing mixing of cold-climate water with higher He, more saline groundwaters.



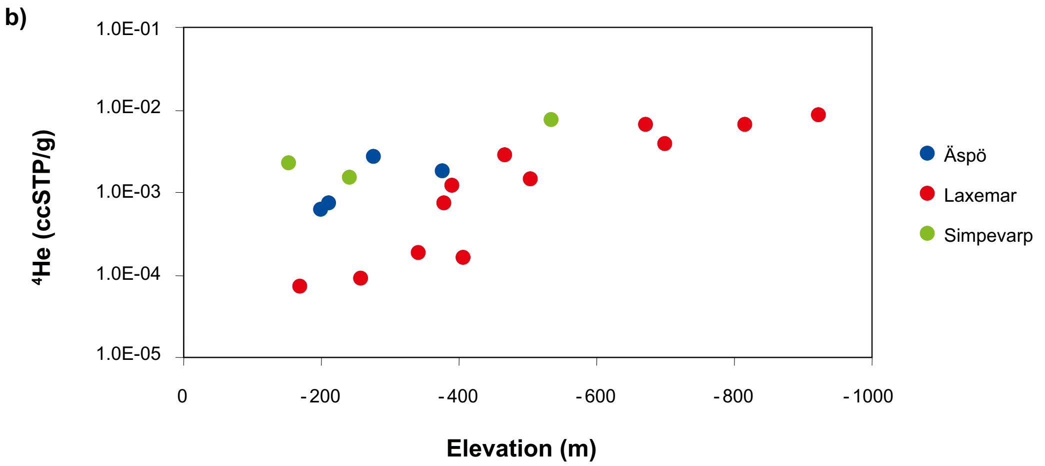


Figure 3-1. a) He concentrations versus Cl in Laxemar/Äspö/Simpevarp groundwaters and b) He concentrations versus depth in Laxemar/Äspö/Simpevarp groundwaters.

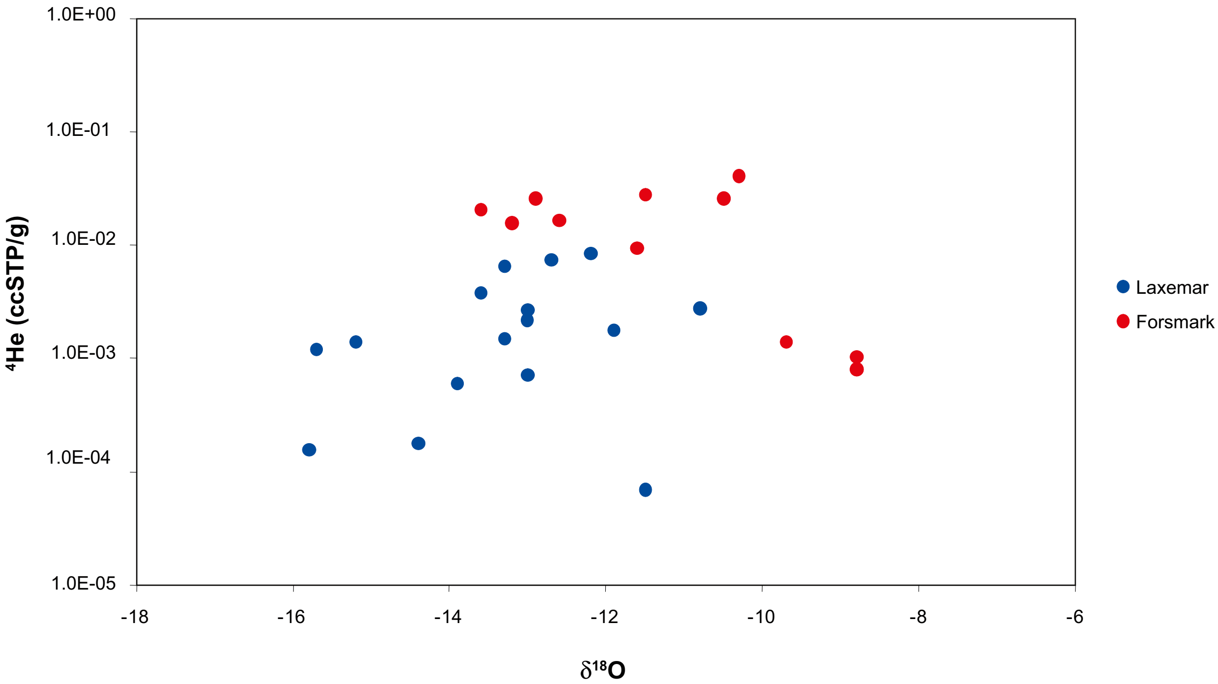


***Figure 3-2.** Variation of He content with $\delta^{18}O$ in Forsmark and Laxemar groundwaters (see text).*

3.2 Chlorine-36

There are only six ^{36}Cl analyses of Laxemar groundwaters from Sicada and five from /Louvat et al. 1999/ (Figures 3-3 and 3-4), and these are listed in Table 3-1a and b together with values for the Forsmark and Olkiluoto sites. Chloride content and zone depth are also shown with the results of accelerator mass spectrometry analysis in Table 3-1b. Ratios of ^{36}Cl/Cl at Laxemar range from high values (76×10^{-15}) for the single, dilute, near-surface sample to low values (1.7×10^{-15}) for the brackish – SO$_4$ samples. This single low value is for a shallow (17 m) groundwater which, nevertheless, has a high Cl concentration (3,660 mg/L). The ^{36}Cl/Cl ratio is close to the detection limits for ^{36}Cl and may be due to minimal mixing with recent infiltration coupled with decay of in situ produced ^{36}Cl as might occur in a groundwater discharge zone. In the dilute sample, ^{36}Cl is probably derived mainly from cosmogenic sources and thus this groundwater could be recent and probably < 50 years old. It is also possible that this sample may contain a small quantity of 'bomb pulse' ^{36}Cl, produced by atmospheric nuclear bomb tests in the 1950's and 1960's or, even, from the Chernobyl accident in 1986.

The deeper (~ 950 m) brackish to saline Laxemar-Simpevarp-Äspö samples have intermediate values of ^{36}Cl/Cl (26 to 48 × 10^{-15}) ratios and this could indicate that these are values typical of in situ production of ^{36}Cl.

Table 3-1a. Results of ^{36}Cl analyses of Forsmark, Simpevarp/Laxemar, Äspö/Laxemar /from Louvat et al. 1999/ and Olkiluoto groundwaters /Gascoyne 2001/ (ratios are $\times10^{-15}$).

Forsmark		Simpevarp/Laxemar		Äspö/Laxemar (Louvat et al., 1999)		Olkiluoto	
Cl	Cl36/Cl	Cl	Cl36/Cl	Cl	Cl36/Cl	Cl	Cl36/Cl
2,780	16	3,660	1.7	0.6	45	30	121.8
53.4	160	39.3	76	508	24	413	15.3
8,160	34	6,570	26	5,340	20	2,760	12.9
7,460	36	7,880	48	12,300	43	4,500	3.5
10,700	41	10,400	32	45,500	40	4,770	4.6
14,700	28	16,800	39			5,400	11.9
						8,400	22.8
						43,000	16.3

Table 3-1b. Depth and origin of the ^{36}Cl analyses of Forsmark /from Smellie et al. 2008/, Simpevarp/Laxemar, and Äspö/Laxemar /from Louvat et al. 1999/.

SITE	IDCODE	SECMID	SKB No	Cl (mg/L)	Cl36_Cl35Cl37	Cl36_Cl35Cl37_ERR	% Error	Origin
FORSMARK	PFM000062		12592	2,780.0	1.60E-014	1.30E-014	82	Baltic Sea
FORSMARK	HFM04	62.00	12704	53.4	1.60E-013	5.00E-014	32	Fresh meteoric recharge water
FORSMARK	KFM08D	831.97	12776	8,160.0	3.40E-014	3.00E-015	9	Brackish non marine groundwater
FORSMARK	KFM08D	673.27	12818	7,460.0	3.60E-014	6.00E-015	16	Brackish non-marine groundwater
FORSMARK	KFM03A	982.00	12711	10,700.0	4.10E-014	4.00E-015	9	Saline groundwater
FORSMARK	KFM07A	967.00	12729	14,700.0	2.80E-014	7.00E-015	25	Saline groundwater
SIMPEVARP	PSM002064	17.00	11515	3,660.0	1.70E-015	1.60E-015	96	Baltic Sea
LAXEMAR	HLX28	80.11	10872	39.3	7.60E-014	5.00E-015	6	Fresh meteoric recharge water
SIMPEVARP	KSH01A	257.50	11494	6,570.0	2.60E-014	4.00E-015	17	Brackish (Littorina) type
LAXEMAR	KLX04	973.71	7753	7,880.0	4.80E-014	4.00E-015	8	Brackish (non-marine) groundwater
LAXEMAR	KLX03	969.83	10077	10,400.0	3.20E-014	4.00E-015	12	Deep saline groundwater
SIMPEVARP	KSH02	957.70	7114	16,800.0	3.90E-014	7.00E-015	19	Deep saline groundwater
Äspö/Laxemar	Local Meteoric	0	Louvat et al. 1999	0.6	45·E-15			Fresh meteoric recharge water
Äspö/Laxemar	KAS04	226	Louvat et al. 1999	508	24·E-15	3·E-15		Shallow fresh groundwater
Äspö/Laxemar	KAS02	314	Louvat et al. 1999	5,340	20·E-15	4·E-15		Brackish (weak Littorina) type
Äspö/Laxemar	KAS03	860	Louvat et al. 1999	12,300	43·E-15	3·E-15		Deep saline groundwater
Äspö/Laxemar	KLX02	1,420	Louvat et al. 1999	45,500	40·E-15	4·E-15		Deep saline groundwater

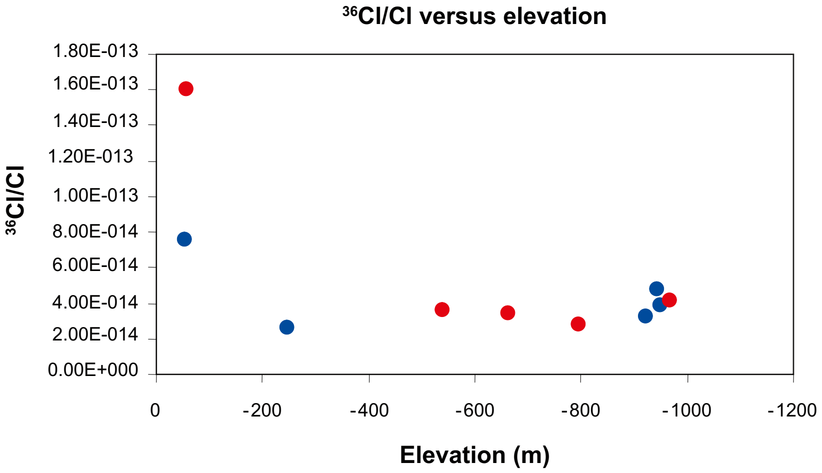


Figure 3-3. Variations of ^{36}Cl/Cl with depth: in blue are Laxemar+Simpevarp data and in red the Forsmark data.

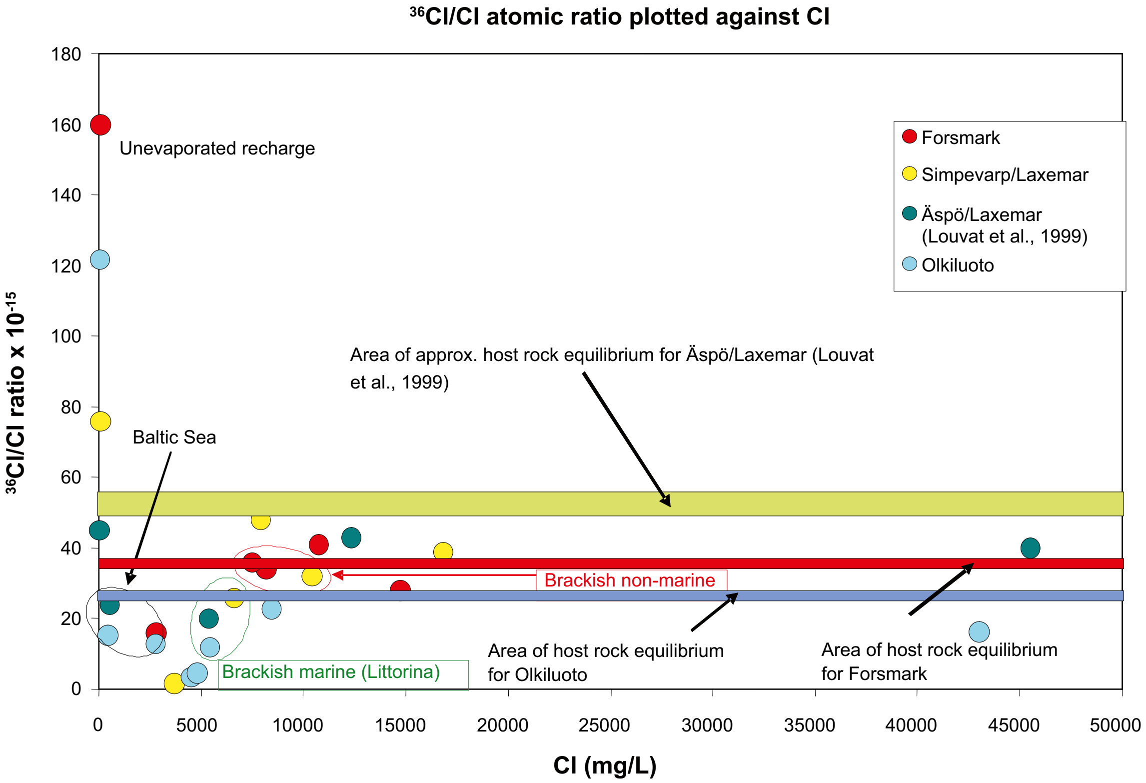


Figure 3-4. Variations of ^{36}Cl/Cl versus Cl /from Smellie et al. 2008/. In red are the Forsmark samples, in yellow are Laxemar+Simpevarp data, in green the Äspö/Laxemar data from /Louvat et al. 1999/ and in light blue the Olkiluoto data.

The variations of ^{36}Cl/Cl with depth and Cl are shown in Figures 3-3 and 3-4, respectively, together with data from Forsmark and other sites. The brackish-Cl and deep saline samples have intermediate ratio values that are slightly higher than other sites. For instance, Olkiluoto has groundwater ^{36}Cl/Cl values of ~ 12 to 23×10^{-15} /Gascoyne 2001/ whereas Laxemar values range from 16 to 48×10^{15}. In these waters, no correlation is seen between the ^{36}Cl/Cl ratio and groundwater Cl concentration (Figure 3-4). This indicates that the surface-derived ^{36}Cl component either has decayed to very low levels or, more probably, been masked by ^{36}Cl produced in situ by (η,γ) reactions with ^{35}Cl present in soluble salts in the rock matrix. This effect has been observed in Canadian Shield groundwaters /Gascoyne et al. 1989/ where studies of the content of soluble salts have shown that Cl in unaltered grey granite exists as salts in micropores (as fluid inclusions) and as grain boundary deposits, which are accessible to permeating groundwater.

The agreement between the two deeper saline groundwaters (Figure 3-4) and the calculated secular equilibrium in situ production line is less constrained than the brackish non-marine groundwaters but is still within the overall uncertainty of the calculations. For both samples, therefore, some mixing with other chloride sources may have occurred during drilling and sampling which may explain the observed small deviations from the in situ production value.

Alternatively, the rocks in which these waters originally reside might have slightly different U, Th, K, Gd, Sm, etc concentrations and thus have a slightly different neutron flux and ^{36}Cl in situ production. For example, the results of neutron calculations performed for Olkiluoto rocks (as described above) are shown here in Table 3-2. Although the rock types and elemental compositions are different to those of Laxemar (or even Forsmark) the variation in ^{36}Cl/Cl values is not large (25–35×$10^{-15)}$ except for one run which has a high REE content and gives a ratio of ~ 10×10^{-15}). Nevertheless, there is no doubt that the intermediate brackish non-marine and deeper saline groundwaters indicate long residence times which reflect early Quaternary times and may even pre-date the Quaternary period.

The Baltic Sea water and the brackish marine (Littorina) groundwater behave interestingly. Both types have ^{36}Cl/Cl ratios below those of the secular equilibrium with granitic rocks and far below those of fresh meteoric recharge (Figure 3-4). If recharge was the dominant water source for these sea waters, then they would have a higher ^{36}Cl/Cl ratio. In contrast, the low ratios measured indicate that most of the chloride dissolved in the Littorina and the Baltic Sea has resided in the bedrock over long periods of time and therefore has been shielded from the atmosphere. That the brackish marine (Littorina) groundwater has a lower ratio than the Baltic Sea water indicates that its dissolved chloride content must have undergone additional shielding from atmospheric input and/or undergone mixing with low ^{36}Cl groundwater from the bedrock. This is consistent with an overall older 'age' of this water type, but not old enough to receive a significant quantity of subsurface-produced ^{36}Cl. In agreement with /Gascoyne 2001/ 'this provides strong support for the argument that these (brackish marine) waters are derived from the Littorina Sea'.

In addition, the consistency of ^{36}Cl/Cl ratios for several widely separated locations and different rock compositions suggests that these groundwaters are in secular equilibrium and, therefore likely to be older than 1.5 million years.

For the brackish to saline non-marine groundwaters it would require about 1.5 Ma to produce the measured ^{4}He concentration in situ. This is in accordance with the ^{36}Cl data for the deep saline groundwaters from both the Forsmark and Laxemar sites where secular equilibrium appears to have been achieved. This is strong evidence that at these depths the average groundwater residence time is indeed in the order of 1.5 Ma. At shallower levels, due to increased fracturing, similar groundwater types might either receive helium from below or from rock alteration processes both of which lead to an overestimation of their residence time.

Table 3-2. Variation of calculated equilibrium $^{36}Cl/Cl$ ratio for in situ production for various concentrations of heavy rare earth elements (HREE) and porosity.

	Base case (8.8 ppm Gd, Sm)			**Low HREE (3 ppm)**			**High HREE (60 ppm)**		
	Mica gneiss	**Tonalite**	**Migmatite**	**Mica gneiss**	**Tonalite**	**Migmatite**	**Mica gneiss**	**Tonalite**	**Migmatite**
Porosity, %	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
ppm U	4.5	3.8	7.8	4.5	3.8	7.8	4.5	3.8	7.8
ppm Th	13.2	11.8	4.9	13.2	11.8	4.9	13.2	11.8	4.9
Yield, n/g/yr/ppm U (= X)	1.128	1.176	1.049	1.128	1.176	1.049	1.128	1.176	1.049
Yield, n/g/yr/ppm Th (= Y)	0.523	0.540	0.481	0.523	0.540	0.481	0.523	0.540	0.481
Total yield, n/g/yr	13.901	12.081	13.867	13.901	12.081	13.867	13.901	12.081	13.867
Thermal cross-section, cm^2/g	0.0072	0.0072	0.00645	0.00598	0.00599	0.00523	0.018	0.018	0.0172
Thermal flux, $n/cm^2/yr$	1,931	1,678	2,150	2,325	2,017	2,651	772	671	806
Equilibrium $^{36}Cl/Cl \times 10^{-15}$	28	24	31	34	29	38	11	10	12

	Base case (0.1% porosity)			**High porosity (1% porosity)**			**Very high porosity (10% porosity)**		
	Mica gneiss	**Tonalite**	**Migmatite**	**Mica gneiss**	**Tonalite**	**Migmatite**	**Mica gneiss**	**Tonalite**	**Migmatite**
Porosity, %	0.1	0.1	0.1	1	1	1	10	10	10
ppm U	4.5	3.8	7.8	4.5	3.8	7.8	4.5	3.8	7.8
ppm Th	13.2	11.8	4.9	13.2	11.8	4.9	13.2	11.8	4.9
Yield, n/g/yr/ppm U (= X)	1.128	1.176	1.049	1.128	1.176	1.049	1.128	1.176	1.049
Yield, n/g/yr/ppm Th (= Y)	0.523	0.540	0.481	0.523	0.540	0.481	0.523	0.540	0.481
Total yield, n/g/yr	13.901	12.081	13.867	13.901	12.081	13.867	13.901	12.081	13.867
Thermal cross-section, cm^2/g	0.0072	0.0072	0.00645	0.00727	0.00728	0.00652	0.00805	0.00805	0.0073
Thermal flux, $n/cm^2/yr$	1,931	1,678	2,150	1,912	1,659	2,127	1,727	1,501	1,900
Equilibrium $^{36}Cl/Cl \times 10^{-15}$	28	24	31	28	24	31	25	22	28

4 Conclusions

Hydraulic properties at depth in the Laxemar site indicate low flow/stagnant groundwater conditions, suggesting residence times that appear to be considerable and are comparable to those from isotopic data. From ^{4}He and ^{36}Cl systematics, the residence time of the brackish to saline non-marine groundwaters can be shown to extend back to at least 1.5 Ma. Groundwaters believed to be derived from Littorina seawater have low ^{36}Cl/Cl ratios and are consistent with other isotopic and geochemical measures of their residence time and with data from other Baltic sites.

Acknowledgements

The authors would like to acknowledge the assistance of Marcus Laaksoharju, John Smellie, Eva-Lena Tullborg, Nick Waber and Bill Wallin in obtaining basic data and providing graphs and diagrams.

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Section 6

Quality assurance and categorisation of groundwater samples from the Laxemar-Simpevarp area

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Contents

Appendix

Preface

This work has been conducted for SKB within the framework of ChemNet, the group responsible for the hydrogeochemical site description of the Laxemar-Simpevarp area. The documented quality assurance and categorisation of the groundwater samples forms a major input to the exploratory analysis and an important base for the modelling part of the Laxemar hydrochemical evaluation /Laaksoharju et al. 2009/.

1 Introduction

The SDM-Site Laxemar hydrochemistry evaluation is based on the 'Extended data freeze Laxemar 2.3' of December 4th, 2007. These data were compiled and their quality checked in February 2008, and the resulting 'internal' dataset was used both for the hydrogeochemical modelling and for delivery to HydroNet. Minor edits and updates were carried out in May 2008 and this version represents the final 'Extended data freeze Laxemar 2.3' dataset used in the SDM-Site Laxemar hydrogeochemistry modelling. Additional data, for example from borehole KLX27A, were compiled in October 2008 but only used for comparison purposes as partial support in the construction of the conceptual visualisations. All datasets are stored in the SKB Simon model database.

The datasets used in the SDM-Site Laxemar hydrochemistry evaluation include all relevant data in the Simpevarp and Laxemar subareas together with available information from Äspö (before the tunnel construction, i.e. the preinvestigation data). The Sicada database contains complete hydrogeochemical analyses including microbes, colloids and gas analysis, and porewater analyses from bedrock samples. In this report the quality assessment of the Laxemar-Simpevarp data is documented together with reference to earlier evaluated Äspö, Ävrö and Simpevarp data. Groundwater data from other Nordic sites and SFR (Final Repository for Radioactive Operational Waste) have been used on occasions for comparison /e.g. Gimeno et al. 2009/. However, these are not included in this document.

2 Borehole groundwater chemistry data

The locations of the percussion and cored boreholes in the Laxemar subarea are shown in Figure 2-1; a total of 46 cored and 43 percussion boreholes have been drilled. Twenty cored boreholes and 19 percussion boreholes were sampled for hydrochemical evaluation, and of the cored boreholes 6 were sampled also for gases, 5 for microbes and 4 for colloids.

Table 2-1 summarises the type and number of samples included in the dataset for the Laxemar and Simpevarp subareas and the data freeze at which they were delivered /Gimeno et al. 2009/.

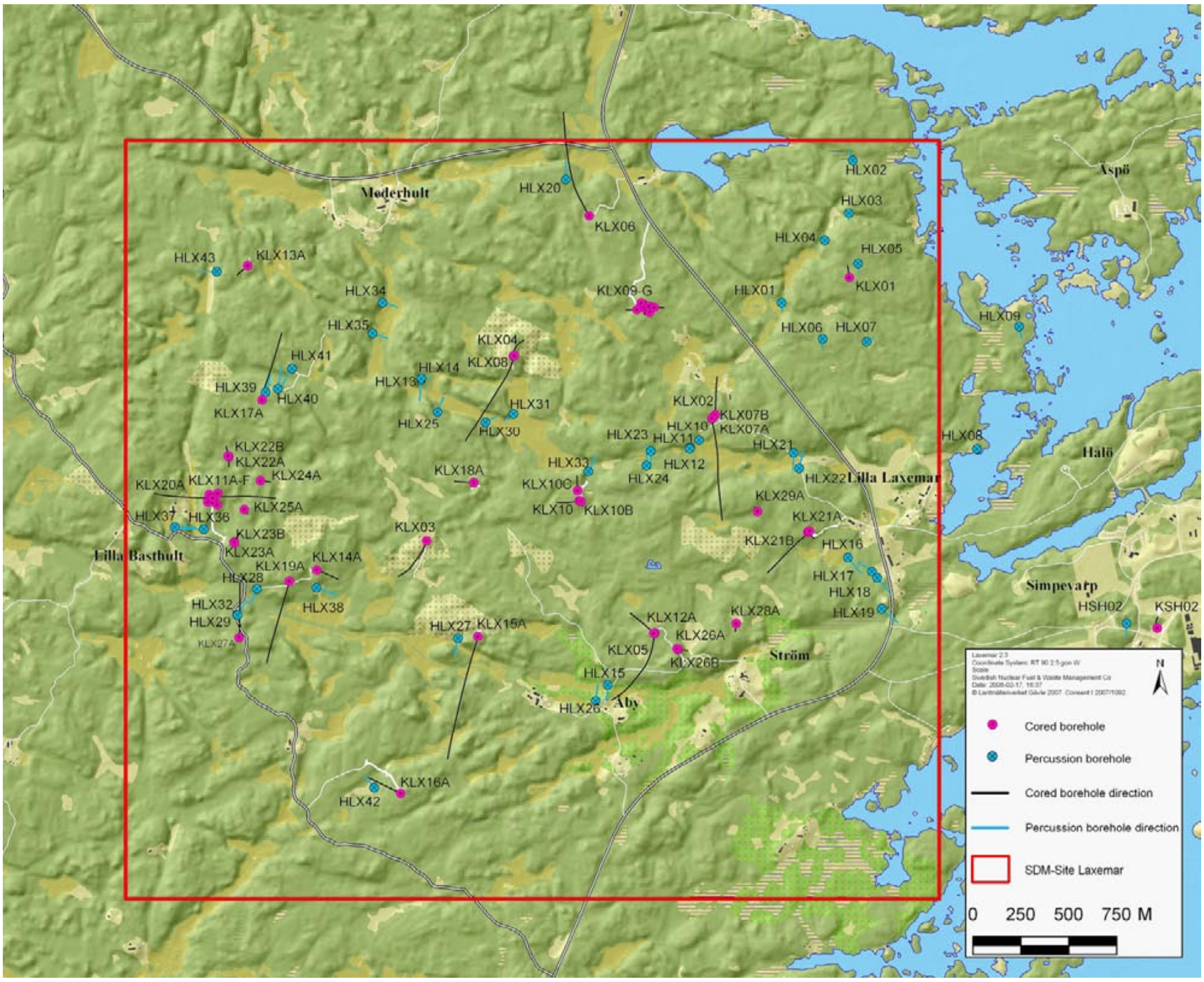

Figure 2-1. Location of the drill sites and boreholes within the Laxemar subarea.

Table 2-1. Number of sampling points and types of sample categories included in the final 'Extended data freeze Laxemar 2.3' for the Laxemar-Simpevarp area. The different rows indicate the number of new samples delivered at each data freeze (2.1, 2.2 and 2.3) or updated existing samples between one data freeze and the next (2.1–2.2 and 2.2–2.3). No supplementary data from existing samples in Laxemar 2.1 and 2.2 were added after the final 'Extended data freeze Laxemar 2.3'. The numbers in the table indicate the total number of sampling points and then after the slash, the number of these sample points which have category 1, 2, 3, or 4. (Perc. Bhs: percussion boreholes; Cored Bhs: cored boreholes; NSGW: near surface groundwaters; Precip: precipitation.)

		Perc. Bhs.	Cored Bhs	Tube Sampling	NSGW	Sea Water	Lake Water	Stream Water	Precip.
Laxemar 2.1	Äspö	14/5	137/21						
	Ävrö		61/3						
	Laxemar	15/5	122/12	35/2	45/39				
	Simpevarp	10/2	15/3	10/0	53/38	54/31	230/186	553/335	
Laxemar 2.1–2.2	Ävrö	9/4	4/0						
	Laxemar	5/3	39/7	64/0	4/4				
	Simpevarp		11/5	20/0	37/22	289/124	17/15	38/32	2/2
Laxemar 2.2	Ävrö		3/0						
	Laxemar	14/6	49/4	46/5					
	Simpevarp		10/2		68/60	67/29	34/34	64/63	3/3
Laxemar 2.2–2.3	Laxemar	3/3	26/6	17/2					
	Simpevarp		2/2		8/6	4/2	2/2	6/6	3/3
Laxemar 2.3	Laxemar	1/1	46/9	4/0					
	Simpevarp				27/21	24/11	13/13	33/31	1/1
Total		71/29	525/74	196/9	242/190	438/197	296/250	694/467	9/9

3 Quality assured data

3.1 Hydrochemical data

The 'Extended data freeze Laxemar 2.3' groundwater dataset has been evaluated systematically with respect to quality, and an assignment of different categories made with respect to their value for further hydrogeochemical interpretational work. This was based on an integrated geological, hydrogeological and hydrochemical approach. A separate small-scale feasibility study of some selected borehole sections was made to determine the possibility of further quantifying the effects from drilling and pumping, Gascoyne and Gurban section #3 this report, but this did not affect the categorisation of the dataset presented here. Of the five categories chosen, Categories 1–3 primarily meet the requirements of hydrogeochemical (but also hydrogeological) modelling, Category 4 primarily meets hydrogeological requirements (but may also be used with caution for more qualitative hydrogeochemical modelling), while Category 5 generally needs to be used with great caution in the context of both hydrogeochemistry and hydrogeology, in particular the tube sampling (or hydrochemical logging) data. A colour code was introduced to quickly distinguish between sample quality when, for example, data are presented in spread-sheet tables or as symbols in scatter plots. In the database, the classification category is indicated numerically in a separate column in addition to the colour coding. An outline of the classification into the various categories for the cored boreholes is presented in Table 3-1. The number of samples and the allocated category are listed in Table 3-2 and the complete tables, mentioned in the Introduction, are stored in the SKB Simon model database.

Table 3-1. Classification criteria for cored boreholes.

Cored Borehole Aspects/Conditions	Category 1	2	3	4	5
Drilling water (≤ 1%)	x	x	x	x	x
Drilling water (≤ 5%)		x	x	x	x
Drilling water (≤ 10%)			x	x	x
Drilling water (> 10%)				x	x
Time series (adequate)	x	x	x	x	x
Time series (inadequate)			x	x	x
Time series absent				x	x
Suitable section length	x	x	x	x	x
Sampling during drilling				x	x
Sampling using PLU hydraulic testing equipment			x	x	x
Tube sampling					x
Charge balance ±5% (±10% for <50 mg/L Cl)	x	x	x	x	x
Major ions (complete)	x	x	x	x	x
Major ions (incomplete)			x	x	x
Environmental isotopes (complete)	x	x	x	x	x
Environmental isotopes (incomplete)		x	x	x	x
Hydraulic effects (short circuiting)					x

Table 3-1 lists the most important criteria used to categorise the groundwater samples. For example, a Category 1 sample has < 1% drilling water, adequate time-series data to assess groundwater chemical stability when sampled, an adequate section length based on the hydraulic properties of the borehole, a charge balance within ±5% (or ±10% for shallow dilute samples), complete major ion and isotope data and, finally, no evidence of short circuiting either within the borehole around the packed-off section or between different fracture systems in the surrounding bedrock. Ideally, these Category 1 groundwaters should also cover microbes, colloids, organics and gases, but these have not been routinely sampled and also require different evaluation criteria. In comparison, a Category 3 sample may have some of the Category 1 criteria but will differ in failing to satisfy all the criteria. For example, the sample may be characterised by inadequate time series data and/or > 5% drilling water. At the other extreme, a Category 5 sample may still record < 1% drilling water and have a complete set of analytical data, but fail to meet several or all of the other criteria, for example, long sampled section, inadequate time-series data and influenced by short circuiting effects etc. Type samples in this category include those collected during drilling and using the PLU hydraulic testing equipment. Almost all samples of tube sample origin also fall within this category because of open hole mixing effects.

It should be noted that the amount of uranine spiked water used for drilling is based on an average value of the uranine. This introduces a degree of uncertainty which may influence the calculated percentage of drilling water for any one borehole section sampled for groundwater. However, this is not considered to be at a level to negatively influence the categorisation procedure.

Table 3-2. Number of samples from percussion and cored boreholes allocated to each category.

Category	1	2	3	4	5
Percussion boreholes	0	0	0	12	3
Cored boreholes	2	3	18	23	242

The main criteria used to categorise the groundwaters sampled from percussion and cored boreholes are:

Category 1 Samples: Characterised by adequate time-series data (i.e. stable chemistry recorded over an adequate time period of days to weeks) and accompanied by complete analytical data (i.e. particularly all major ions and environmental isotopes); a charge balance of ±5% (or ±10% for more dilute groundwaters) and less or close to 1% drilling water; absence of ^{14}C and/or $\delta^{13}C$ values is accepted in groundwaters with HCO_3 contents less than 20 mg/L. In addition, reliable redox values; a good coverage of trace elements (including U, Th and REEs), and, if possible, microbe, organic and dissolved gas data, is also recommended. Note, however, that the quality of these last mentioned parameters is not considered in the categorisation because they require a different set of criteria.

Category 2 Samples: Of similar quality to Category 1 but marked by incomplete analytical data (usually restricted to an absence of ^{14}C and $\delta^{13}C$ and less trace element, microbe, organic and gas data) and/or with elevated concentrations of drilling water (1 to 5%).

Category 3 Samples: This category differs from Categories 1 and 2 in terms of inadequate time-series data; time-series data that indicate instability during sampling; incomplete analytical data (such as absence of some isotopic and trace element data, microbe, organic and gas data, and redox values); elevated drilling water concentrations (5 to 10%).

Category 4 Samples: Analyses are mostly restricted to Cl, Br, $\delta^{18}O$, Mg, HCO_3, Na, Ca, SO_4; elevated drilling water concentrations (> 10%); absence or very incomplete (i.e. inadequate) time-series data. Type samples are often of an exploratory nature, i.e. mostly taken to see if there is adequate water volume and to check strategic indicators such as drilling water content, salinity (electrical conductivity) ± pH ± major ions (Cl, Br, SO_4, HCO_3) ± $\delta^{18}O$. Some samples taken during drilling and often those sampled using PLU hydraulic testing equipment fall within this category unless not specifically classified as Category 5.

Category 5 Samples: Samples with some major ions or $\delta^{18}O$ missing; no charge balance values; elevated drilling water concentrations (> 10%); absence or very incomplete (i.e. inadequate) time-series data. Type samples in this category include those collected during drilling and those sampled using PLU hydraulic testing equipment. Most samples of tube sample (or hydrochemical logging) origin also fall within this category because of open hole mixing effects. Note, however, that in some cases the uppermost tube sample (usually near surface groundwater from highly transmissive zones) and the deepest sample (usually the most saline accumulation due to density constraints) may be quite representative.

The highest quality data are required, for example, for geochemical equilibrium calculations, modelling of redox conditions, and reliability for specialised studies involving microbes, organics and colloids. On the other hand overall site understanding (e.g. groundwater distribution, origin and evolution and its integration with hydrogeology) is adequately addressed by a combination of all categories with the obvious proviso that the higher the category number of data used, the more caution is required in their interpretation.

As a general rule, samples classified as category 1 to 4 data have been used mainly in the presentation and interpretation of the SDM-Site Laxemar modelling. However, there are occasions where it can be very helpful to plot initially all data, for example, for ^{18}O and tritium, to obtain a general impression of site behaviour and follow this up using only category 1 to 3 or 1 to 4 data to quantify interpretation and description. On other occasions it is important to trace the evolution of a specific analysis over the set time period of sampling, and for this the whole time series of measurements have been used to derive, for example, field measurements of pH and Eh which may not be available for the actual sample selected as being most representative hydrochemically. The lack of such field data has reduced considerably the available set of samples for speciation-solubility calculations.

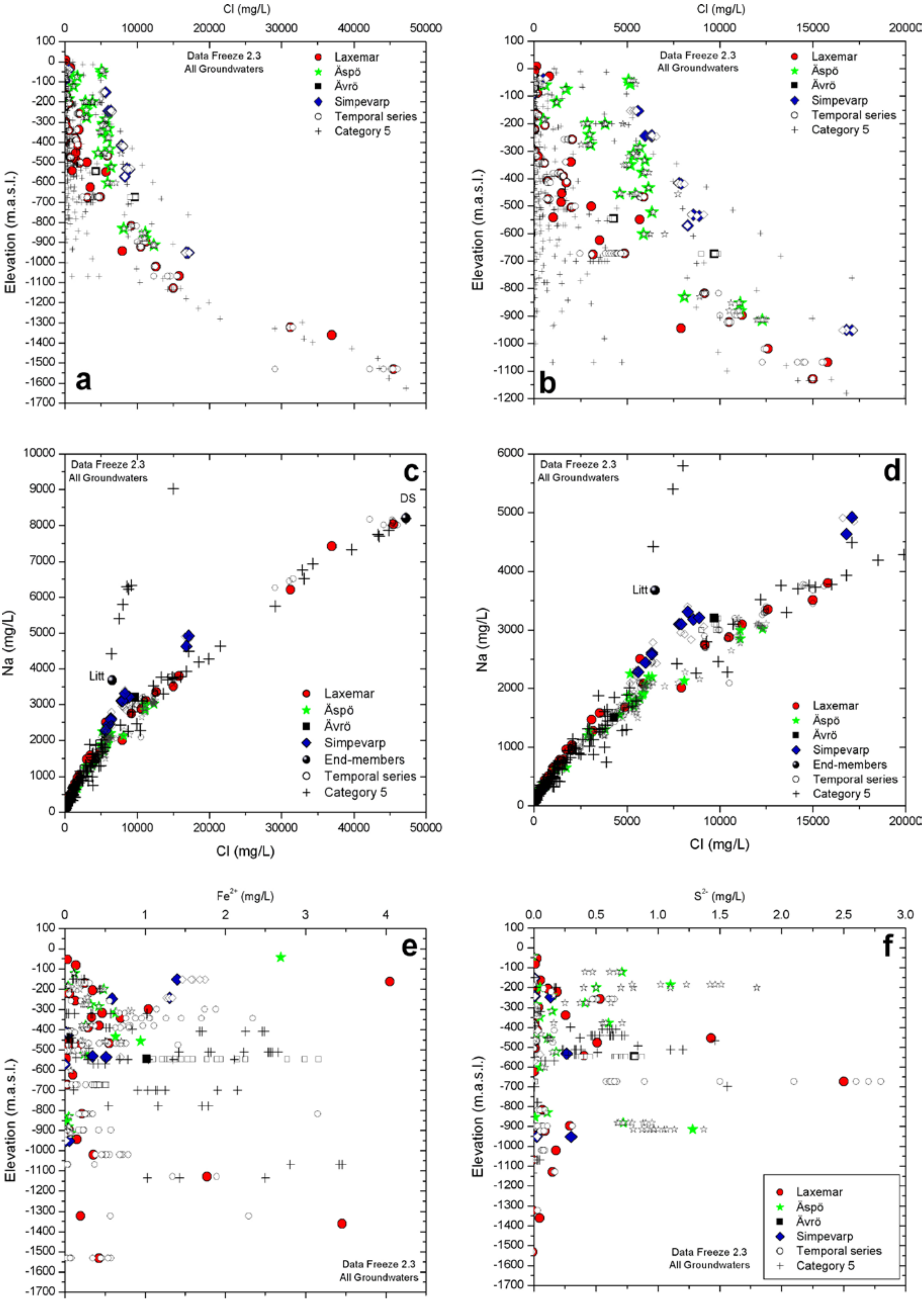

Figure 3-1. *Examples of trends shown by groundwaters representing all sample categories (1 to 4 are colour coded) and including time-series variations. Plots (b) and (d) are the same as (a) and (c) respectively, but with the x-axis enlarged to better visualise the shallow to intermediate depths /Gimeno et al. 2009/.*

Analysed data include the same parameters chosen in the previous Laxemar 2.1 hydrogeochemical model version. The pH, Eh, temperature and conductivity values used in this report are the ones determined in the field when available (i.e. from Chemmac logs). In the remaining cases, laboratory determinations have been included in the table but not used for modelling purposes.

In order to observe the effects or consequences of using a selected set of category 1 to 3 or 1 to 4 samples instead of all samples, a comparative analysis has been made. Figure 3-1 plots all the samples, i.e. including samples from category 5 and also time-series samples. The main conclusions from this comparison are that:

- In most cases, the absence of category 5 samples greatly enhances the general trends derived from the category 1 to 4 samples. In some cases, however, the presence of category 5 samples serves to cover gaps when there is a shortage of higher quality category 1–4 samples.
- Samples corresponding to the time series measurements (open symbols in Figure 3-1) usually plot at the same position as the samples selected as representative for the sampled section. For example, in the case of chloride or sodium (Figure 3-1a and b), i.e. indicative for the major ions, the differences found related to different samples taken from the same depths are negligible.
- For ferrous iron and sulphide and including trace elements in general, samples based on time-series measurements (and the monitoring programme) usually show a range of variation which could be expected as they are very sensitive to the sampling procedures.
- Samples categorised as 5 include tube samples, samples collected during drilling and samples generally with high drilling water content.

3.1.1 Questionable data

Some data appear to be reasonably representative but they may still reflect a wide range of possible influences on groundwater flow conditions. These include; a) limited hydraulic short circuiting effects during sampling, b) small scale contamination from different borehole activities, and c) induced mixing over large distances by long term draw-down hydraulic pumping tests and dilution and tracer tests. Some issues of concern were identified which included:

- The hydraulic tracer test programme involved at different stages from 2003 to 2007 the injection of uranine (and additionally caesium and rubidium in six tests) in boreholes KLX01, KLX02, KLX03, KLX04, KLX05, KLX06, KLX07A, KLX10A, KLX11A and KLX18A. In some of the sampled groundwaters, especially from monitoring sections, this has resulted in an increase of uranine, which may be incorrectly interpreted as an artefact of the introduced uranine (as a flushing water tracer) during initial drilling of the boreholes. Furthermore, some of the monitoring samples showed anomalous increases in caesium and in these cases the tested borehole sections were identified and documented.
- Low but detectable tritium contents (around one or a few TU) have been detected at varying depths in the Laxemar subarea in many cases where it would not otherwise be expected. In instances where contamination due to excess drilling water or normal tritiated shallow formation groundwaters could be excluded, the risk of artificial contamination, therefore, had to be addressed. For some of the samples the problem was found subsequently to have originated from a leakage of tritium from the down-hole pumping equipment where high tritium in deionised water is occasionally used during routine Complete Chemical Characterisation (CCC) sampling. For other sections there is no clear cut explanation, but i*n situ* production of tritium in the bedrock and laboratory contamination where considered less probable.

- During sampling, fracture networks intersecting the boreholes may lead to short circuiting of the groundwater flow in the surrounding bedrock and also to bypassing the packer systems used to isolate the borehole sections being sampled (Figure 3-2). This effectively means that the section sampled may have been supplied by mixed groundwaters from higher or lower levels in the bedrock, and/or mixed borehole waters above or below the packer systems. In both cases the sampled groundwaters when interpreted in isolation may be evaluated erroneously as being of high quality. Short circuiting is indicated by either '?' or 'x?' in the attached categorisation tables Appendices A–D where they indicate 'possible short circuiting' or 'likely short circuiting' respectively.

Each of these issues have been addressed in detail during the quality evaluation of the data and appropriate action taken in the categorisation process.

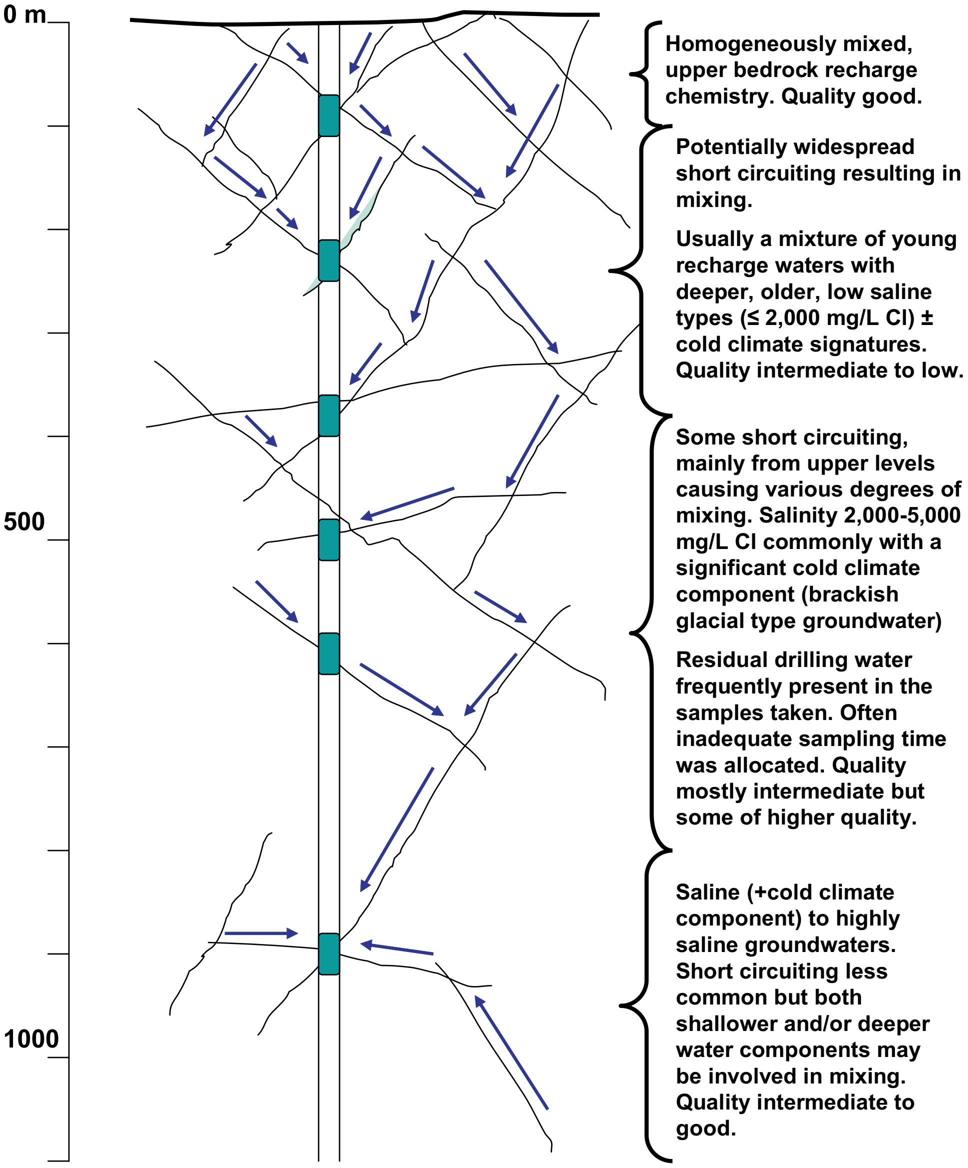

Figure 3-2. *Schematic illustration of a generalised Laxemar subarea borehole showing the result of potential perturbations from borehole activities and the corresponding quality of groundwater sampled at different depths.*

3.2 Appendix structure

The appendix part of this section is structured to first present and categorise for each site the percussion borehole hydrochemical data and then the cored borehole data; earlier documentation is outlined in /Smellie and Laaksoharju 1992, SKB 2006a and b/.

Documentation of the percussion boreholes and sites already evaluated (i.e. Äspö, Ävrö and Simpevarp) is restricted mainly to tabular form accompanied by a brief description of the hydrochemistry of the drilling water and the major category criteria that characterise the groundwater chemistry from each sampled borehole length or isolated borehole section. The cored borehole documentation of the Laxemar subarea, in addition to the category table, is accompanied by a description of: a) the general hydraulic and hydrochemical character of the borehole and the packed-off sections sampled, b) the hydrochemistry of the drilling water, c) the major ion and isotope chemistry, and c) the reasoning behind the different categories selected.

Unless otherwise stated, all metric reference to the depth, length and sampling location along the boreholes is in 'borehole length' and not vertical depth or elevation.

4 References

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SKB, 2006b. Hydrogeochemical evaluation – Preliminary site description Laxemar subarea – version 2.1. SKB R-06-70, Svensk Kärnbränslehantering AB.

Äspö preinvestigation data (1987–1989)

A1 Percussion boreholes

A1.1 HAS02 (44.0-93.0 m; mid. vertical elevation: –56.41 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)			x		
Section without flow log (0–100 m)					
Time series/monitoring			x		
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)			?		

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –0.42% to +0.98%

Time Series: Two samples over a period of 2 days. Salinity shows a slight instability (decrease) from 5,470–5,160 mg/L Cl; longer time-series data required. Incomplete major ions: no Fe^{2+}, Mn, S^{2-} and TOC.

Isotopes: Incomplete isotopes; no carbon isotopes; tritium below detection limit (< 1 TU); $\delta^{18}O$ values about –7.7‰ VSMOW typical of a significant marine component.

Trace elements: Lack of data.

General: Overall salinity range, the presence of significant Mg (217–244 mg/L) and SO_4 (155–162 mg/L) and the enriched $\delta^{18}O$ values all signify a typical brackish marine-type groundwater (Littorina), sometimes present at this shallow depth.

Comment: Limited time series and lack of Fe^{2+}, absence of trace element data and the possibility of short circuiting (~ 50 m near surface borehole length). Allocated Category 3.

A1.2 HAS03 (48.0–100.0 m; mid. vertical elevation: –60.36 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)			x		
Section without flow log (0–100 m)					
Section without flow log (0–200 m)					
Time series/monitoring			x		
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)			?		

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –1.48% to –0.26%.

Time Series: Two samples over a period of 2 days. Salinity indicates stability (574–608 mg/L Cl). Incomplete major ions: no Fe^{2+}, Mn, S^{2-} and TOC.

Isotopes: Incomplete isotopes; no carbon isotopes; tritium at 33–35 TU; $\delta^{18}O$ values (around –10.8‰ VSMOW) typify recharge conditions.

Trace elements: Lack of data.

General: Weak brackish groundwater ($Na\text{-}HCO_3(Cl)$) type) with Mg present at 36–39 mg/L (due to a weak marine component) and Ca at 80–87 mg/L. There is the possibility of some short circuiting (~ 50 m near surface borehole length).

Comment: Limited time series, lack of Fe^{2+}, Mn, S^{2-} and TOC and the absence of carbon isotpes and trace element data. Allocated Category 3.

A1.3 HAS05 (45.0–100.0 m; mid. vertical elevation: –56.35 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)				x	
Section without flow log (0–100 m)					
Section without flow log (0–200 m)					
Time series/monitoring				x	
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)				?	

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –1.17% to +1.3%.

Time Series: Two samples over a period of 2 days. Salinity indicates stability (119–123 mg/L Cl). Incomplete major ions: no Br, Fe^{2+}, Mn, S^{2-} and TOC.

Isotopes: Incomplete isotopes; no carbon isotopes; tritium below detection (< 1 TU) to 2 TU; $\delta^{18}O$ values (about –9.8‰ VSMOW) typify recharge conditions.

Trace elements: Lack of data.

General: Fresh groundwater ($Na\text{-}HCO_3(Cl)$) type with low Mg (4–6 mg/L) and Ca (25–27 mg/L) with a modern component indicated by the presence of tritium. Typical near surface groundwaters although there is the possibility of some short circuiting (~ 55 m near surface borehole length).

Comment: Limited time series, absence of Br, Fe^{2+}, Mn, S^{2-} and TOC and trace element data. Allocated Category 4.

A1.4 HAS06 (40.0–100.0 m; mid. vertical elevation: –65.05 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					x
Section without flow log (0–200 m)					
Time series/monitoring					x
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					?

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at +0.72% to +0.94%

Time Series: Two samples over a period of 2 days. Cl shows marked instability (280–1,760 mg/L) accompanied by an increase in Mg (11–56 mg/L). Incomplete major ions: Br (one value at 7 mg/L) and Fe^{2+}, Mn, S^{2-} and TOC absent.

Isotopes: Incomplete isotopes; no carbon isotopes; tritium variable from 24–11 TU and $\delta^{18}O$ from –10.2 to –9.4‰ VSMOW.

Trace elements: Lack of data.

General: Change from a mainly fresh water to a brackish marine-type groundwater with time, probably due to an increasing Littorina-type water supported by more enriched $\delta^{18}O$, an increase in Mg from 11–56 mg/L and Na from 254–900 mg/L. The decrease in tritium indicates a more deeper-derived groundwater source.

Comment: Unstable time series, absence of Fe^{2+}, Mn, S^{2-} and TOC and the absence of trace element data point to a major uncertainty in representativity. This is also coupled with probable short circuiting within the sampled 60 m borehole length. Allocated Category 5.

A1.5 HAS07 (71.0–100.0 m; mid. vertical elevation: –75.06 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length			x		
Section with flow log					
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					
Section without flow log (0–200 m)					
Time series/monitoring			x		
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)			?		

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –2.04% to –0.33%

Time Series: Two samples over a period of 2 days. Salinity indicates some instability (1,650–1,740 mg/L Cl) accompanied by small increases in Mg (48–55 mg/L) and SO_4 (116–122 mg/L). Incomplete major ions: no Fe^{2+}, Mn, S^{2-} and TOC absent.

Isotopes: Incomplete isotopes; no carbon isotopes; tritium below detection (< 1 TU) and $\delta^{18}O$ values stable at –11.2 to –11.3‰ VSMOW.

Trace elements: Lack of data.

General: Groundwater is weakly brackish with a possible marine component influence which appears to increase with time. Even though a fairly restricted borehole length has been sampled (29 m), short circuiting is suggested to explain this increase.

Comment: Limited time series, no Fe^{2+}, Mn, S^{2-} and TOC, and the absence of trace element data. However, at the time of sampling the groundwater is considered fairly representative for this shallow level. Allocated Category 3.

A1.6 HAS13 (0–100.0 m; mid. vertical elevation: –42.64 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)					
Section without flow log (0–100 m)			x		
Section without flow log (0–200 m)					
Time series/monitoring			x		
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)			x?		

Charge Balance: No measured values given in Sicada but modelled PHREEQC values for the final two groundwaters sampled are +1.48% and +0.43% respectively.

Time Series: Four samples over a period of 4 days. Salinity indicates small instability (5,360–5,100 mg/L Cl) accompanied by a small decrease also in Mg (243–216 mg/L) and increase in SO_4 (117–142 mg/L). Incomplete major ions characterise the initial two samples and the final sample, i.e. absence of Fe^{2+}, Mn and TOC. For the third, most complete analysis, the major ions are complete apart from TOC.

Isotopes: Only analysed for the third sample where they are incomplete: no carbon isotopes; tritium at 1.2 TU, and $\delta^{18}O$ at –7.2‰ VSMOW indicating a significant marine component.

Trace elements: Lack of data.

General: Sample is a typical brackish marine (Littorina-type) groundwater Na(Ca, Mg)-Cl(HCO_3,SO_4) which has undergone some dilution during the four day sampling period.

Comment: Lack of time series data, absence of Fe^{2+}, Mn and TOC and groundwater sampled from a long (100 m) borehole section introduces uncertainty, but otherwise the sample is close to a representative Littorina-type groundwater not uncommon in the upper bedrock. Allocated Category 3.

A2 Cored boreholes

A2.1 KAS02 (202.00–214.59 m; mid. vertical elevation: –199.81 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)			x		
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)			x		
Time series (inadequate)					
Time series absent					
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO_3(Cl) fresh groundwater with chloride at 119 mg/L, with $\delta^{18}O$ at –9.9‰ VSMOW and δ^2H at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –2.18% to +1.19%.

Time Series: 1988-12-16 to 1989-01-11. Adequate time series with initial instability in salinity for the first 2 days (4,770–3,280 mg/L Cl) and then stable for the rest of the sampling period (3,820–3,740 mg/L Cl). This stability is reflected by the other major ions (Na, Ca, Mg, HCO_3 and SO_4). Drilling water is consistently < 1% apart from the first sample taken (3%). Complete major ions apart from TOC.

Isotopes: Isotope data only available for the final sample collected and this lacks carbon isotopes. Tritium at 0.3 TU for the last sample, and $\delta^{18}O$ at –13.90‰ VSMOW indicates a significant cold climate component.

Trace elements: Lack of data.

General: Dominant Na-Ca-Cl groundwater with significant cold climate and marine components.

Comment: Good stable composition, no indication of short circuiting, but missing time series for the isotopes + absence of carbon isotopes + absence of trace element data. In general, however, groundwater typical of what would be expected at this depth. Allocated Category 3.

A2.2 KAS02 (314.00–319.00 m; mid. vertical elevation: –307.69 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)			x		
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)			x		
Time series (inadequate)					
Time series absent					
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO_3(Cl) fresh groundwater with chloride at 119 mg/L, with $\delta^{18}O$ at –9.9‰ VSMOW and $\delta^{2}H$ at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –2.53% to +2.25%

Time Series: 1988-03-25 to 1988-04-12 (18 days). Adequate time series showing reasonably consistent stability in salinity throughout the sampling period although a small decrease with time is noted (5,550–5,340 mg/L Cl); last two days stable at 5,340 mg/L Cl. This decrease reflects a small increase in Mg (58–75 mg/L) and HCO_3 (24–27 mg/L). Drilling water consistently < 1%. Complete major ions apart from TOC.

Isotopes: Incomplete isotopes; no carbon isotopes. Only one sample analysed for tritium at 8 TU (detection limit at this time), and $\delta^{18}O$ at –12.3‰ VSMOW possibly indicates a weak cold climate signature.

Trace elements: Lack of data.

General: Dominant Na-Ca-Cl groundwater with potentially some weak traces of cold climate and marine (i.e. Mg presence) components.

Comment: Good stable composition but missing time series for the isotopes, absence of carbon isotopes and absence of trace element data. In general, however, groundwater typical of what would be expected at this depth. Allocated Category 3.

Note: *Section 308.00–344.00 m in KAS02 (mid. vertical elevation: –326.00 m) comprising 5 samples collected 5 months later, shows an identical groundwater chemistry and the last sample collected is allocated a Category 3.*

A2.3 KAS02 (463.00–468.00 m; mid. vertical elevation: –456.16 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)			x		
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)			x		
Time series (inadequate)					
Time series absent					
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO_3(Cl) fresh groundwater with chloride at 119 mg/L, with $\delta^{18}O$ at –9.9‰ VSMOW and δ^2H at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –3.19% to +1.59% except for the two early stage samples not considered at –33.55% and –5.71% (i.e. samples 1421, 1422)

Time Series: 1988-04-13 to 1988-04-25 (12 days). Adequate time series (7 samples); initial sample not considered. Not all data are complete (e.g. K and Mg) but available data show consistent stability in salinity throughout the sampling period (5,370–5,520 mg/L Cl); drilling water consistently < 1%. For the chosen sample major ion data complete apart from TOC.

Isotopes: Incomplete isotopes; only data for the final sample. No ^{14}C (low HCO_3 < 30 mg/L), $\delta^{13}C$ at –6.5‰ PDB. Tritium below detection (8 TU limit at this time), and $\delta^{18}O$ at –12.8‰ VSMOW indicates a cold climate component.

Trace elements: Lack of data.

General: Dominant Na(Ca)-Cl(SO_4) brackish groundwater with weak cold climate and marine components (Mg at 66–67 mg/L).

Comment: Good stable composition but missing time series for some major ions and isotopes. Absence of trace element data + high tritium detection limit restricts evaluation. In general terms, however, groundwater typical of what would be expected at this depth. Allocated Category 3.

A2.4 KAS02 (530.00–535.00 m; mid. vertical elevation: –522.95 m)

Cored Borehole **Category**	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)			x		
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)			x		
Time series (inadequate)					
Time series absent					
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO_3(Cl) fresh groundwater with chloride at 119 mg/L, with $\delta^{18}O$ at –9.9‰ VSMOW and δ^2H at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values indicate the first two samples as unsuitable (–35.38% and –35.26%; samples 1429 and 1430) and the remaining 3 samples suitable at –1.89% to –0.2%.

Time Series: 1988-04-28 to 1988-05-05 (7 days) with limited time series (3) when excluding the first two samples. However, reasonable stability in salinity is suggested for the sampling period (6,330–6,410 mg/ Cl); drilling water consistently < 1%. For the chosen sample major ion data complete apart from an absence of TOC.

Isotopes: Incomplete isotopes; no carbon isotopes (lack of $HCO_3 \sim 10$ mg/L). For the final sample tritium is under detection (8 TU detection limit at this time), and $\delta^{18}O$ at –12.3‰ VSMOW suggests a weak cold climate component.

Trace elements: Lack of data.

General: Dominant Na(Ca)-Cl(SO_4) brackish groundwater with weak cold climate and marine components (Mg at 42 mg/L).

Comment: Few major ion data but stable composition indicated during the final sampling period and < 1% drilling water. The few major ion data + no trace element data + high tritium detection limit, all restrict evaluation. In general terms, however, groundwater typical of what would be expected at this depth. Allocated a Category 3.

A2.5 KAS02 (802.00–924.04 m; mid. vertical elevation: –852.33 m)

Cored Borehole **Category**	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)			x		
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)			x		
Time series (inadequate)					
Time series absent					
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)			x		

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO_3(Cl) fresh groundwater with chloride at 119 mg/L, with $\delta^{18}O$ at –9.9‰ VSMOW and $\delta^{2}H$ at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –3.16% to –2.00%.

Time Series: 1988-09-17 to 1988-09-20 (3 days). Moderate time series (4 samples) but not all data available for all samples (i.e. Mg and K). Available data show a small consistent increase in salinity with time (10,600–11,100 Cl), reflected also with small increases in Na, Ca and SO_4. Drilling water consistently < 1%. Major ion data incomplete apart for the final sample collected (exception TOC).

Isotopes: Incomplete isotopes; no carbon isotopes (lack of HCO_3^- ~ 7 mg/L). For the final sample tritium is at 8 TU (detection limit at this time) and $\delta^{18}O$ at –13.0‰ VSMOW indicates a significant cold climate component.

Trace elements: Lack of data.

General: Dominant Ca(Na)-Cl(SO_4) brackish non-marine groundwater (mineralisation increasing slightly with time) with a significant cold climate signature. However, a weak marine component with Mg at 31 mg/L is suggested.

Comment: Few major ion data and unstable composition indicated with a small but consistent increase in mineralisation with time (short circuiting?). Absence of trace element data, high tritium detection limit and a long borehole section (122 m) that can facilitate short circuiting, all restrict evaluation. In general terms, however, groundwater typical of what would be expected at this depth and with < 1% drilling water. Allocated Category 3.

A2.6 KAS02 (860.00–924.04 m; mid. vertical elevation: –881.22 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)			x		
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)			x		
Time series (inadequate)					
Time series absent					
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)			?		

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO$_3$(Cl) fresh groundwater with chloride at 119 mg/L, with δ^{18}O at –9.9‰ VSMOW and δ^2H at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –2.26% to +1.87% (exception is the first sample 1549 at –24.71% which is excluded).

Time Series: 1989-01-13 to 1989-01-31 (18 days). Adequate time series (11 samples) showing consistent stability in salinity throughout the sampling period (at 10,500–11,100 mg/L Cl). Drilling water consistently < 1%. Major ion data complete (TOC and DOC under detection).

Isotopes: Incomplete isotopes; no carbon isotopes (lack of HCO$_3^-$ < 12 mg/L). For the final and only sample tritium is virtually absent at 0.2 TU (which may be an indication that previous values at shallower depths could also be much lower), and δ^{18}O at –13.1‰ VSMOW indicates a significant cold climate component.

Trace elements: Lack of data.

General: Dominant Ca(Na)-Cl(SO$_4$) brackish non-marine groundwater with a significant cold climate component. However, a weak marine component is suggested (Mg at about 31 mg/L).

Comment: Good stable composition but missing time series for the isotopes, no trace element data and a long borehole section (64 m) that can facilitate short circuiting, all restrict evaluation. In general terms, however, groundwater typical of what would be expected at this depth. Allocated Category 3.

A2.7 KAS03 (129.00–134.00 m; mid. vertical elevation: –121.78 m)

Cored Borehole **Category**	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)			x		
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)			x		
Time series (inadequate)					
Time series absent					
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO_3(Cl) fresh groundwater with chloride at 119 mg/L, with $\delta^{18}O$ at –9.9‰ VSMOW and δ^2H at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –2.39% to +0.56%.

Time Series: 1989-02-07 to 1989-02-21 (14 days). Adequate time series (9 samples) showing consistent stability in salinity throughout the sampling period (1,210–1,240 mg/L Cl). Drilling water consistently < 1%. Major ion data almost complete; exception Fe^{2+} for the first 4 samples and TOC for all samples.

Isotopes: Incomplete isotopes; no carbon isotopes. For the final and only sample tritium is at 0.1 TU, and $\delta^{18}O$ at –15.8‰ VSMOW indicates a significant cold climate component.

Trace elements: Lack of data.

General: Dominant Na(Ca)-Cl(HCO_3) brackish glacial groundwater with a significant cold climate signature.

Comment: Good stable composition. However, missing time series for the isotopes + incomplete major ions + absence of carbon isotopes and no trace element data, all restrict evaluation. In general terms, however, groundwater typical of what would be expected at this depth. Allocated Category 3 for the final sample.

A2.8 KAS03 (196.00–222.00 m; mid. vertical elevation: –198.73 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)				x	
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)				x	
Time series absent					
Suitable section length				x	
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO_3(Cl) fresh groundwater with chloride at 119 mg/L, with $\delta^{18}O$ at –9.9‰ VSMOW and δ^2H at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –2.81% to –0.10%.

Time Series: 1988-08-07 to 1988-08-10 (3 days). Inadequate time series (4 samples) although there is consistent stability in salinity throughout the short sampling period (2,850–2,920 mg/L Cl) when excluding the first sample. Drilling water is inconsistent (2.7–8.43%). Major ion data incomplete with sporadic values of K, Br and HCO_3 and an absence of Fe(tot), Fe^{2+}, Mn, S^{2-} and TOC in all but the final sample in which there was an absence in Fe(tot), Fe^{2+} and TOC.

Isotopes: Incomplete isotopes; no carbon isotopes. For the final and only sample tritium is at 8 TU (detection limit at this time), and $\delta^{18}O$ at –14.6‰ VSMOW indicates a significant cold climate component.

Trace elements: Lack of data.

General: Dominant Na(Ca)-Cl brackish glacial groundwater with a possible weak marine component (Mg ~ 60 mg/L).

Comment: Few data but stable composition although missing time series for the isotopes, absence of carbon isotopes, high tritium detection limit, no trace element data and a high uncertain drilling water content, all restrict evaluation. Last sample taken has the most complete data but missing drilling water content (indications are low) + no Fe(tot), Fe^{2+} and TOC. In general terms, however, groundwater typical of what would be expected at this depth. Allocated Category 4 for the final sample.

A2.9 KAS03 (248.00–251.00 m; mid. vertical elevation: –238.92 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)			x		
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)			x		
Time series absent					
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)			?		

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO_3(Cl) fresh groundwater with chloride at 119 mg/L, with $\delta^{18}O$ at –9.9‰ VSMOW and δ^2H at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –1.5% to 0.83%.

Time Series: 1988-08-26 to 1988-08-28 (2 days). Inadequate time series (3 samples) which suggest a small decrease in salinity (3,010–2,950 mg/L Cl) accompanied by a decrease in Ca and SO_4 and small increase in Mg (54–58 mg/L). Drilling water shows a consistent decrease from 2.68–1.04%. Major ion data incomplete with sporadic measurements of Fe(tot), Fe^{2+} and S^{2-}, with TOC and DOC under detection.

Isotopes: Incomplete isotopes; no carbon isotopes. For the final and only sample tritium is below detection (< 8 TU, i.e. detection limit at this time), and $\delta^{18}O$ at –14.5‰ VSMOW indicates a significant cold climate component.

Trace elements: Lack of data.

General: Dominant Na(Ca)-Cl brackish glacial groundwater with a significant cold climate component and a minor marine component (Mg ~ 55 mg/L).

Comment: Inadequate time series, no time series for the isotopes, absence of carbon isotopes, high tritium detection limit, no trace element data and uncertain final drilling water content, all restrict evaluation. Short circuiting is also a possibility. Last sample taken has most data but missing certain parameters (i.e. no Fe(tot) and Fe^{2+} although his can be extrapolated from preceding samples). In general terms, however, groundwater typical of what would be expected at this depth. Allocated Category 3 for last sample.

A2.10 KAS03 (347.00–373.00 m; mid. vertical elevation: –348.56 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)			x		
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)			x		
Time series absent					
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)			x?		

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO$_3$(Cl) fresh groundwater with chloride at 119 mg/L, with δ^{18}O at –9.9‰ VSMOW and δ^{2}H at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –2.7% to –1.15%

Time Series: 1988-08-13 to 1988-08-16 (4 days). Inadequate time series (4 samples) showing a small but progressive increase in salinity (4,810–5,180 mg/L Cl), accompanied by increases in Na, Ca and SO$_4$; only one Mg value is recorded (40 mg/L). Drilling water shows a consistent decrease during sampling period (7.89–0.83%). Major ion data incomplete (e.g. no Fe(tot) or Fe^{2+}) and K, Mg and S^{2-} are only sporadically analysed during the series; TOC and DOC are under detection.

Isotopes: Incomplete isotopes; no carbon isotopes (lack of HCO$_3$ ~ 13 mg/L). For the final and only sample tritium is below detection (< 8 TU, i.e. detection limit at this time) and δ^{18}O at –13.3‰ VSMOW indicates a significant cold climate component.

Trace elements: Lack of data.

General: Dominant Na-Ca-Cl(SO$_4$) brackish glacial groundwater with decreased Mg compared the preceding two samples (but still with a possible weak marine component?), and a cold climate component.

Comment: Inadequate time series, no time series for the isotopes, high tritium detection limit and no trace element data, all restrict evaluation. Short circuiting is suspected. Last sample taken has most data but missing certain parameters (i.e. no Fe(tot), Fe^{2+} and TOC). In general terms, however, groundwater typical of what would be expected at this depth. Allocated Category 3 for the final sample with < 1% drilling water.

A2.11 KAS03 (453.00–480.00 m; mid. vertical elevation: –454.25 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)			x		
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)			x		
Time series absent					
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO_3(Cl) fresh groundwater with chloride at 119 mg/L, with $\delta^{18}O$ at –9.9‰ VSMOW and δ^2H at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –2.95% to +0.31%

Time Series: 1988-08-19 to 1988-08-22 (4 days). Inadequate time series (4 samples) but Cl in the last two samples suggests an approach to stability (~ 4,600 mg/L), which is reflected by Ca, Mg, HCO_3 and SO_4. Drilling water shows a consistent decrease during the sampling period (3.62–2.13%). Major ion data incomplete with respect to Fe(tot), Fe^{2+} and Mn; TOC and DOC are under detection.

Isotopes: Incomplete isotopes; no carbon isotopes (Lack of HCO_3 ~ 30 mg/L). For the final and only sample tritium is below detection (< 8 TU, i.e. detection limit at this time) and $\delta^{18}O$ at –13.6‰ VSMOW indicates a significant cold climate component.

Trace elements: Lack of data.

General: Dominant Na(Ca)-Cl(SO_4) brackish glacial groundwater with a possible weak marine component, similar Mg (~ 40 mg/L) and cold climate signature to the preceding sample.

Comment: Inadequate time series so a degree of uncertainty of final stable composition; stability eventually suggested but drilling water > 1%. Missing time series for the isotopes, absence of carbon isotopes, high tritium detection limit and no trace element data, all restrict evaluation. Last sample taken has most data but missing certain parameters (i.e. no Fe(tot), Fe^{2+} and TOC); data from the preceding sample can be used. In general terms, however, groundwater typical of what would be expected at this depth. Allocated Category 3 for the final sample.

A2.12 KAS03 (609.00–623.00 m; mid. vertical elevation: –602.45 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)			x		
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)			x		
Time series absent					
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)			?		

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO_3(Cl) fresh groundwater with chloride at 119 mg/L, with $\delta^{18}O$ at –9.9‰ VSMOW and $\delta^{2}H$ at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –1.75% to +0.56%

Time Series: 1988-08-31 to 1988-09-03 (4 days). Inadequate time series (4 samples); progressive decrease in salinity (7,020–5,880 mg/L Cl) which is reflected by Ca, Mg, HCO_3 and SO_4. Drilling water shows also a consistent decrease during sampling period (3.92–2.23%). Major ion data sporadic and incomplete with respect to Fe(tot), Fe^{2+}, Mn and TOC.

Isotopes: Incomplete isotopes; no carbon isotopes (lack of HCO_3 ~ 11 mg/L). For the final and only sample tritium is below detection (< 8 TU, i.e. detection limit at this time) and $\delta^{18}O$ at –13.3‰ VSMOW indicates a significant cold climate component.

Trace elements: Lack of data.

General: Dominant Na(Ca)-Cl(SO_4) brackish glacial groundwater with little change in Mg (38 mg/L) from the preceding sample.

Comment: Inadequate time series so a degree of uncertainty of final stable composition (short circuiting?); drilling water still decreasing (> 1%). Missing time series for the isotopes, high tritium detection limit and no trace element data, all restrict evaluation. Last sample taken has most data but missing certain parameters (i.e. no Fe(tot), Fe^{2+} and TOC); data from the preceding sample can be used. In general terms, however, groundwater typical of what would be expected at this depth. Allocated Category 3 for the final sample.

A2.13 KAS03 (690.00–1002.06 m; mid. vertical elevation: –829.97 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)			x		
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)			x		
Time series absent					
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)			x?		

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO_3(Cl) fresh groundwater with chloride at 119 mg/L, with $\delta^{18}O$ at –9.9‰ VSMOW and $\delta^{2}H$ at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –4.74% to –2.62%.

Time Series: 1988-09-06 to 1988-09-08 (2 days). Inadequate time series (3 samples); small decrease in salinity (8,900–8,080 mg/L Cl) not reflected by the other major ions (lack of data). Drilling water shows a small but consistent decrease during sampling period (2.92–2.57%). Major ion data sporadic and incomplete with respect to Fe(tot), Fe^{2+} and Mn; TOC and DOC are under detection.

Isotopes: Incomplete isotopes; no carbon isotopes (lack of HCO_3 ~ 11–13 mg/L). For the final and only sample tritium is below detection (< 8 TU, i.e. detection limit at this time), and $\delta^{18}O$ at –13.0‰ VSMOW indicates a significant cold climate component.

Trace elements: Lack of data.

General: Change to a dominant Ca(Na)-Cl(SO_4) brackish glacial groundwater with a slightly greater Mg content (~ 45 mg/L) compared to the preceding sample indicating a possible weak marine component.

Comment: Inadequate time series in general; 2 samples in the final 2 days show potential stable composition but also missing time series for the isotopes,high tritium detection limit and no trace element data, all restrict evaluation. Furthermore, a long borehole length (~ 312 m) was sampled which may have contributed to a homogenisation of the groundwaters prior to sampling and /or short circuiting. Last sample taken has most data but missing certain parameters (i.e. Fe(tot) Fe^{2+}), although these can be extrapolated from the preceding samples. In general terms, however, this groundwater is typical of what would be expected at this depth. Allocated Category 3 for the final sample.

A2.14 KAS03 (860.00–1002.06 m; mid. vertical elevation: –914.01 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)			x		
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)			x		
Time series (inadequate)					
Time series absent					
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)			x		
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)			x?		

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO_3(Cl) fresh groundwater with chloride at 119 mg/L, with $\delta^{18}O$ at –9.9‰ VSMOW and $\delta^{2}H$ at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –1.43% to +0.78%

Time Series: 1989-02-24 to 1989-03-15 (20 days). Adequate time series (13 samples) with stabilisation of salinity (homogenisation?) indicated by Cl (and the other major ions) being achieved after the first 7 days (12,200–12,300 mg/L) following a small increase from 12,100 to 12,500 mg/L Cl. Drilling water consistently < 1%. Major ion data complete; below detection for TOC/DOC.

Isotopes: Complete isotopes; no carbon isotopes (lack of HCO_3 ~ 11 mg/L). For the final and only sample tritium is very low at 0.4 TU and $\delta^{18}O$ at –12.7‰ VSMOW indicates a very weak cold climate component.

Trace elements: Lack of data.

General: Dominant Ca(Na)-Cl(SO_4) brackish groundwater with consistent Mg (~ 50 mg/L) suggesting a possible weak marine component together with a weak glacial signature .

Comment: Adequate time series in general, but also missing data for the isotopes combined with no trace element data which restrict evaluation. Furthermore, a long borehole length (~ 142 m) was sampled which may have contributed to a homogenisation of the groundwaters prior to sampling and/or facilitated short circuiting. Last sample taken has most measured data. In general terms, however, groundwater typical of what would be expected at this depth. Allocated Category 3 for the final sample.

A2.15 KAS04 (102.00–202.00 m; mid. vertical elevation: –118.52 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					x
Drilling water (> 10%)					x
Time series (adequate)					
Time series (inadequate)					x
Time series absent					
Suitable section length					
Sampling during drilling					x
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO_3(Cl) fresh groundwater with chloride at 119 mg/L, with $\delta^{18}O$ at –9.9‰ VSMOW and $\delta^{2}H$ at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –2.68% to –0.82%

Time Series: 1989-04-16. Sampled during drilling; inadequate time series (2 samples) indicate salinity instability (1,150–754 mg/L Cl), reflected by the other major ions. Drilling water decreased rapidly from 67.6–6.6% during the sampling. Major ion data incomplete; absence of Fe(tot), Fe^{2+}, S^{2-}, Mn, Li, Sr, TOC and DOC.

Isotopes: Lack of data.

Trace elements: Lack of data.

General: Ca(Na)-Cl(HCO_3,SO_4) brackish water mixture.

Comment: Sampling during drilling and a long borehole section (~ 100 m), possibly facilitating short circuiting, all resulting in a mixing of groundwaters from different sources and a large component of drilling water. Inadequate and unreliable data to determine sample status. Allocated Category 5 for the final sample.

A2.16 KAS04 (202.00–325.00 m; mid. vertical elevation: –212.72 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					x
Drilling water (> 10%)					x
Time series (adequate)					
Time series (inadequate)					x
Time series absent					
Suitable section length					
Sampling during drilling					x
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO_3(Cl) fresh groundwater with chloride at 119 mg/L, with $\delta^{18}O$ at –9.9‰ VSMOW and δ^2H at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –2.14% to 0.52%.

Time Series: 1989-02-26. Sampled during drilling; inadequate time series (2 samples) although salinity remained quite stable (1,310–1,290 mg/L Cl) supported by the other major ions. Drilling water decreased from 65.6–53.6%. Major ion data incomplete; absence of Fe(tot), Fe^{2+}, S^{2-}, Mn, Li, Sr, TOC and DOC.

Isotopes: Lack of data.

Trace elements: Lack of data.

General: Dominant Ca(Na)-Cl(HCO_3,SO_4) brackish groundwater with consistent Mg (~ 30 mg/L) which may suggest a minor marine component.

Comment: Inadequate time series, no isotopes, no trace element data, incomplete major ions and very high drilling water, all restrict evaluation. Sampled during drilling and possible short circuiting have resulted mostly in a mixture of drilling water, fresh meteoric water and deeper brackish groundwater homogenised in the long section (123 m) sampled. Inadequate and unreliable data to determine sample status and therefore allocated Category 5 for the final sample.

A2.17 KAS04 (226.00–235.00 m; mid. vertical elevation: –185.14 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)			x		
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)			x		
Time series (inadequate)			x		
Time series absent					
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)			x?		

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO_3(Cl) fresh groundwater with chloride at 119 mg/L, with $\delta^{18}O$ at –9.9‰ VSMOW and δ^2H at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –1.44% to +0.57%.

Time Series: 1989-04-06 to 1989-04-17 (11 days). Adequate time series (8 samples) with close to salinity stabilisation achieved after the first 4 days (635–606 mg/L Cl) followed by a small but consistent decrease in Cl during the rest of the sampling period from 553–508 mg/L Cl. This consistent change is reflected by the other major ions with Na, Ca and Mg showing small decreases and HCO_3 a corresponding increase. Drilling water consistently < 1%. Major ion data complete apart from an absence of TOC and only 1 DOC value for the final sample.

Isotopes: Incomplete isotopes; no carbon isotopes. For the final and only sample tritium is at 4.3 TU and $\delta^{18}O$ at –11.0‰ VSMOW, both indicating a recent recharge groundwater.

Trace elements: Lack of data.

General: Dominantly a Na-Cl(HCO_3,SO_4) brackish groundwater of shallow origin.

Comment: Adequate time series for major ions, but absence of time series for the isotopes, absence of carbon isotopes and no trace element data, all restrict evaluation. Last sample taken has most data but still lacking in Mn, Li and TOC, although the former two ions can be extrapolated from the previous time series values. In general terms, however, perhaps the groundwater is typical of that expected at this depth considering dynamic recharge conditions. Some short circuiting cannot be ruled out. Allocated Category 3 for final sample.

A2.18 KAS04 (334.00–343.00 m; mid. vertical elevation: –275.61 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)			x		
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)			x		
Time series (inadequate)					
Time series absent			x		
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)			x?		

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO_3(Cl) fresh groundwater with chloride at 119 mg/L, with $\delta^{18}O$ at –9.9‰ VSMOW and δ^2H at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –0.15% to +0.71%.

Time Series: 1989-04-19 to 1989-04-27 (10 days). Adequate time series (7 samples) with some instability in salinity during the first 2 days (2,520–2,660 mg/L Cl) and then stable values for the rest of the sampling period (2,920–3,030 mg/L Cl). Stability is supported by the other major ions. Drilling water consistently < 1%. Major ion data almost complete; no TOC and only one DOC value.

Isotopes: Incomplete isotopes; no carbon isotopes. For the final and only sample tritium is at 0.5 TU, and $\delta^{18}O$ at –13.0‰ VSMOW indicates a significant cold climate component.

Trace elements: Lack of data.

General: Dominantly a Na(Ca)-Cl(HCO_3,SO_4) brackish glacial groundwater of upper bedrock origin with a cold climate signature and possibly a weak marine component (Mg ~ 30 mg/L).

Comment: Adequate time series in general, but the absence of time series for the isotopes, absence of carbon isotopes and no trace element data, all restrict evaluation. Last sample taken has most data. The groundwater is considered typical of what would be expected at this depth, considering dynamic recharge conditions. Some short circuiting cannot be ruled out. Allocated Category 3 for final sample.

A2.19 KAS04 (440.00–480.98 m; mid. vertical elevation: –376.74 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)			x		
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)			x		
Time series (inadequate)					
Time series absent			x		
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO_3(Cl) fresh groundwater with chloride at 119 mg/L, with $\delta^{18}O$ at –9.9‰ VSMOW and $\delta^{2}H$ at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –0.84% to +0.76%.

Time Series: 1989-03-22 to 1989-04-03 (12 days). Adequate time series (6 samples) showing stable salinity values (excluding the first sample) for the sampling period (5,990–5,840 mg/L Cl), supported by the other major ions. Drilling water consistently < 1%. Major ion data almost complete; no TOC and only 1 DOC value.

Isotopes: Incomplete isotopes; no carbon isotopes (low HCO_3 ~ 20 mg/L). For the final and only sample tritium records 0.03 TU and $\delta^{18}O$ at –11.9‰ VSMOW.

Trace elements: Lack of data.

General: Dominantly a Na(Ca)-Cl(SO_4) brackish groundwater with Mg (57–61 mg/L) suggesting a marine (Littorina) influence, stronger than indicated in the preceding more shallow groundwater level.

Comment: Adequate time series in general, but missing time series for the isotopes and no trace element data. Last sample taken has best data. In general terms, this groundwater is considered typical of that expected at this depth and therefore allocated Category 3 for final sample.

A2.20 KAS06 (204.00–277.00 m; mid. vertical elevation: –200.01 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					x
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					x
Time series (inadequate)					x
Time series absent					
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO$_3$(Cl) fresh groundwater with chloride at 119 mg/L, with δ^{18}O at –9.9‰ VSMOW and δ^{2}H at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –4.20% to –0.86%.

Time Series: 1989-05-29 to 1989-06-01 (4 days). Inadequate time series (4 samples) to achieve stability; Cl indicates a consistent decrease (4,800–3,310 mg/L) supported by decreases in Na, Ca, Mg and SO$_4$ and an increase in HCO$_3$. Drilling water systematically decreased from 1.19–0.72%. Major ion data incomplete with sporadic Fe(tot), Fe^{2+} and DOC (no TOC recorded).

Isotopes: Incomplete isotopes; no carbon isotopes. For the second last and only sample tritium is at 3.8 TU and δ^{18}O at –10.9‰ VSMOW.

Trace elements: Lack of data.

General: Dominantly a Na(Ca)-Cl(SO$_4$) brackish groundwater with significant Mg (72–118 mg/L) and HCO$_3$ (~ 90 mg/L) indicating a marine (Littorina and/or Baltic Sea) influence.

Comment: Inadequate time series in general, combined with missing time series for the isotopes, absence of carbon isotopes, incomplete major ions and no trace element data, all restrict evaluation. Instability of major ions suggests a short circuiting effect (aided by a long borehole section of 73 m) drawing in less saline younger water (suggested by the tritium content) from shallower levels with time. The sampled groundwater is likely to represent a mixed variety not representative for this level and therefore allocated Category 5.

A2.21 KAS06 (304.00–377.00 m; mid. vertical elevation: –284.27 m)

Cored Borehole **Category**	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)			x		
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)			x		
Time series absent					
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)			?		

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO_3(Cl) fresh groundwater with chloride at 119 mg/L, with $\delta^{18}O$ at –9.9‰ VSMOW and $\delta^{2}H$ at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –1.9% to –0.58%.

Time Series: 1989-06-05 to 1989-06-08 (3 days). Inadequate time series (4 samples); apart from a lower salinity in the initial sample (5,540 mg/L Cl), the salinity appears to have stabilised with time (5,660–5,710 mg/L Cl), together with the other major ions, but more monitoring would have been desirable. Drilling water is consistently < 1% showing a small decrease during sampling from 0.33–0.03%. Major ion data sporadic for Fe(tot) and Fe^{2+} but otherwise complete apart for no TOC and only one DOC value for the second last sample taken.

Isotopes: Incomplete isotopes; no carbon isotopes. For the second last and only sample tritium records 0.3 TU, and $\delta^{18}O$ at –9.2‰ VSMOW is enriched, suggesting a marine component.

Trace elements: Lack of data.

General: Dominantly a Na(Ca)-Cl(SO_4) brackish groundwater with significant Mg (114–119 mg/L), HCO_3 (~ 50 mg/L) and enriched $\delta^{18}O$ indicating a marine component (Littorina-type). This also confirms the suggestion of 'weak Littorina/Baltic' component from the preceding level.

Comment: Inadequate time series in general, combined with missing time series for the isotopes, absence of carbon isotopes, no trace element data and a long borehole section (73 m) which often contributes to groundwater short circuiting and mixing. Nevertheless, considered to be a good example of a Littorina-type groundwater with adequate evidence of being representative for this depth and therefore allocated Category 3.

A2.22 KAS06 (389.00–406.00 m; mid. vertical elevation: –331.84 m)

Cored Borehole **Category**	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)			x		
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)			x		
Time series absent					
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO_3(Cl) fresh groundwater with chloride at 119 mg/L, with $\delta^{18}O$ at –9.9‰ VSMOW and $\delta^{2}H$ at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –1.36% to –0.88%.

Time Series: 1989-06-12 to 1989-06-15 (4 days). Adequate time series (4 samples) indicating stable salinity during the sampling period (5,930–5,970 mg/L Cl), supported by the other major ions. Drilling water consistently < 1% showing a small decrease during sampling from 0.24–0.03%. Major ion data incomplete due to an absence of Fe(tot), Fe^{2+} and TOC; only 1 DOC for the second last sample taken.

Isotopes: Incomplete isotopes; no carbon isotopes. For the second last and only sample, tritium is at 0.6 TU, and $\delta^{18}O$ enriched at –7.40‰ VSMOW again suggests a significant Littorina component.

Trace elements: Lack of data.

General: Dominantly a Na(Ca)-Cl(SO_4) brackish marine (Littorina) groundwater with significant Mg (150–153 mg/L) and HCO_3 (~ 65 mg/L) and enriched $\delta^{18}O$.

Comment: Adequate time series in general, but the missing time series for the isotopes, absence of carbon isotopes and no trace element data, all restrict evaluation. Otherwise a good example of a Littorina-type groundwater representative for this depth and therefore allocated a Category 3.

A2.23 KAS06 (439.00–602.17 m; mid. vertical elevation: –433.02 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)				x	
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)				x	
Time series (inadequate)					
Time series absent					
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)				x	
Major ions (incomplete)					
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)				?	

Drilling water: HAS05 (45.00–100.00 m; mid. vertical elevation: –56.35 m). There is one documented drilling water sample in the Extended L.2.3 dataset from approximately the time of drilling borehole KAS02, i.e. sample collected in 1987-08-07 and used here. Na-HCO_3(Cl) fresh groundwater with chloride at 119 mg/L, with $\delta^{18}O$ at –9.9‰ VSMOW and δ^2H at –73.8‰ VSMOW, and tritium at 2 TU.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –1.6% to +0.4%.

Time Series: 1989-06-19 to 1989-06-22 (3 days). In this case adequate time series (4 samples) indicating stable salinity during the sampling period (6,140–6,170 mg/L Cl) supported by the other major ions. Drilling water consistently < 1% showing a small decrease during sampling from 0.15–0.05%. Major ion data incomplete due to sporadic absence of Fe(tot) and Fe^{2+} and a general absence of TOC; only DOC for the second last sample is recorded.

Isotopes: Incomplete isotopes; no carbon isotopes. For the second last and only sample, tritium at 3.5 TU and $\delta^{18}O$ enriched at –8.2‰ VSMOW again suggests a significant Littorina component.

Trace elements: Lack of data.

General: Dominantly a Na(Ca)-Cl(SO_4) brackish marine (Littorina-type) groundwater with significant Mg (119–130 mg/L) and HCO_3 (~ 50 mg/L); slightly higher salinity, lower Mg and less enriched $\delta^{18}O$ compared to the preceding sample suggest the 'dilution' of the brackish marine (Littorina) groundwater by mixing of a deeper non-marine brackish component. This could have been facilitated by the long borehole length sampled (~ 163 m).

Comment: Adequate time series in general, but missing time series for the isotopes, absence of carbon isotopes, no trace element data and a long borehole section which often facilitates mixing, in this case possibly with a deeper, more saline brackish non-marine groundwater. The high tritium is not easy to explain – possibly contamination by some younger, shallow water component (short circuiting?). Otherwise little difference between this sample and the preceding sample although a greater increase in salinity and a weaker Littorina signature might have been expected with increasing depth. The absence of a sharper transition is thought to reflect the long borehole section sampled. Allocated Category 4.

Appendix B

Ävrö data

B1 Percussion boreholes

B1.1 HAV04 (35.00–100.00 m; mid. vertical elevation: –51.25 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)					
Section without flow log (0–100 m)				x	
Section without flow log (0–200 m)					
Time series/monitoring				x	
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at +3.68% to +4.97%.

Time Series: 1987-07-25 to 1987-07-26 (2 days). Inadequate time series (2 samples) although saline stability (106–108 mg/L Cl) supported by the other major ions. Incomplete major ions; no Br, F, Si, Fe^{2+}, Mn, S^{2-}, Li, Sr and TOC.

Isotopes: Incomplete isotopes; no carbon isotopes. Tritium decreased from 8 TU to below detection (< 1 TU) during sampling, and $\delta^{18}O$ values at –10.1 to –9.9‰ VSMOW.

Trace elements: Lack of data.

General: Na-HCO_3(Cl,SO_4) fresh meteoric groundwater with initially high tritium being reduced to below detection in the second sampling occasion.

Comment: Inadequate time series and lack of important major ions, absence of trace element data, no carbon isotopes and a 65 m borehole length probably facilitating mixing/short circuiting. Allocated Category 4.

B1.2 HAV05 (50.00–100.00 m; mid. vertical elevation: –55.79 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)					
Section without flow log (0–100 m)				x	
Section without flow log (0–200 m)					
Time series/monitoring				x	
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at +1.12% to +1.90%.

Time Series: 1987-07-28 to 1987-07-29 (2 days). Inadequate time series (2 samples); fresh water with Cl at 14–15 mg/L and Mg at 2.0–3.0 mg/L. Incomplete major ions; no Br, F, Si, Fe^{2+}, Mn, S^{2-}, Li, Sr and TOC.

Isotopes: Incomplete isotopes; no carbon isotopes. Tritium decreased from 11 TU to below detection (< 1 TU) during sampling, and $\delta^{18}O$ at –9.80‰ VSMOW.

Trace elements: Lack of data.

General: Na-HCO_3(SO_4) fresh meteoric groundwater of recent origin with initially high tritium being reduced to below detection during the second sampling occasion.

Comment: Inadequate time series and lack of important major ions, absence of trace element data, no carbon isotopes and a 65 m borehole length, probably facilitating mixing/short circuiting. Allocated Category 4.

B1.3 HAV06 (73.00–100.00 m; mid. vertical elevation: –62.80 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)			x		
Section without flow log (0–100 m)					
Section without flow log (0–200 m)					
Time series/monitoring			x		
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole sections					
Hydraulic effects (short circuiting)			?		

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at +0.15% to +98%.

Time Series: 1987-07-30 to 1987-07-31 (2 days). Inadequate time series (2 samples); fresh water with Cl at 22–36 mg/L and Mg at 1.0–1.4 mg/L. Incomplete major ions; no Br, F, Si, Fe^{2+}, Mn, S^{2-}, Li, Sr and TOC.

Isotopes: Incomplete isotopes; no carbon isotopes. Tritium below detection (< 1 TU), and $\delta^{18}O$ at –10.0 to –10.2‰ VSMOW.

Trace elements: Lack of data.

General: Na-HCO_3(SO_4) fresh meteoric groundwater of recent origin.

Comment: Problems include inadequate time series and lack of important major ions, absence of trace element data, no carbon isotopes, and a long (27 m) borehole length that may have facilitated mixing/short circuiting. However, because of an absence of tritium, and a groundwater composition expected at such near surface, a Category 3 is allocated.

B1.4 HAV07 (69.00–100.00 m; mid. vertical elevation: –70.45 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)					
Section without flow log (0–100 m)				x	
Section without flow log (0–200 m)					
Time series/monitoring				x	
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole sections					
Hydraulic effects (short circuiting)				x?	

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –2.58% to –2.24%.

Time Series: 1987-07.29 to 1987-07-30 (2 days). Inadequate time series (2 samples); fresh water with Cl at 63–73 mg/L and Mg at 2.0 mg/L. Incomplete major ions; no Br, F, Si, Fe(tot), Fe^{2+}, Mn, S^{2-}, Li, Sr and TOC.

Isotopes: Incomplete isotopes; no carbon isotopes. Tritium at 2 TU to below detection (< 1 TU) and $\delta^{18}O$ at –10.2 to –9.9‰ VSMOW.

Trace elements: Lack of data.

General: Na-HCO_3(SO_4) fresh meteoric groundwater of recent origin.

Comment: Problems include inadequate time series and lack of important major ions, absence of trace element data, no carbon isotopes, and a long (27 m) borehole length that may have facilitated mixing/short circuiting. Short circuiting is suggested by traces of tritium in the second sample indicating contamination from shallower, even more modern recharge waters. Allocated Category 4.

B1.5 HAV09 (15.00–130.00 m; mid. vertical elevation: –65.48 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					
Section without flow log (0–200 m)					x
Time series/monitoring					
Time series absent					x
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole sections					
Hydraulic effects (short circuiting)					x?

Charge Balance: Sicada measured value at +4.05%.

Time Series: 2003-10-16 (1 day). Absent time series (1 sample); brackish water with Cl at 2,561 mg/L Cl with significant Mg (80.5 mg/L) and SO_4 (69 mg/L) but low HCO_3 (~ 32 mg/L). Incomplete major ions; no Fe(tot), Fe^{2+}, S^{2-}, TOC and DOC.

Isotopes: Lack of data.

Trace elements: Lack of data.

General: Na(Ca)-Cl(SO_4) brackish groundwater with a possible marine component (80.5 mg/L Mg).

Comment: No time series, incomplete major ions, absence of trace element data, no isotope data and a long borehole length (115 m) probably facilitating mixing/short circuiting. Allocated Category 5.

B2 Cored boreholes

B2.1 Borehole KAV01

Borehole KAV01 was drilled in the northeastern part of Avrö island prior to the site characterisation of the Laxemar-Simpevarp area and upgraded so it could be integrated in the Oskarshamn site investigation database. The borehole was therefore drilled in three stages: a) to 502.20 m from 1977-04-21 to 1977-05-16, b) 502.20 to 744.60 m from 1986-10-08 to 1986-11-16, and c) 744.60 to 757.31 m from 1986-11-25 to 1986-11-27 m. The borehole is near-vertical (–89.20° to the horizontal) and cased to 70.04 m.

B2.1.1 KAV01 (391.00–434.00 m; mid. vertical elevation: –398.31 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					x
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					x
Time series (inadequate)					
Time series absent					
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					x
Major ions (incomplete)					
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring section					x
Hydraulic effects (short circuiting)					x?

Charge Balance: Sicada measured values at –1.35% to +0.88%.

Time Series: 2005-11-15 to 2006-10-31 (11.5 months). Adequate time series in terms of intervals (3 samples). Unstable salinity indicated between sampling periods (269–546 mg/L Cl) supported by increases in the other major ions apart for HCO_3 which is fairly constant at 197–228 mg/L. Drilling water consistently < 1%. Major ion data incomplete for the first and third sampling occasion (no Fe(tot), Fe^{2+}, S^{2-}, TOC and DOC), but complete for the second occasion.

Isotopes: Incomplete isotopes; no carbon isotopes. Tritium ranges from 8.2–8.9TU and $\delta^{18}O$ from –10.8 to –11.3‰ VSMOW.

Trace elements: Good coverage for second sampled occasion.

General: Na(Ca)-Cl(HCO_3) weakly brackish non-marine groundwater.

Comment: Adequate time interval series in general with adequate coverage of major and trace elements, but absence of carbon isotopes for all sampled occasions. Groundwater salinity is unstable with time with a general small increase in Cl, Mg and also a small increase in $\delta^{18}O$ depletion. Drilling water contents are potentially problematic because of hydraulic tracer tests carried out from 2005-11-23 to 2005-11-28 in the same borehole section using uranine, i.e. between the first and second groundwater sampling occasions. However, the low uranine content contents exclude any significant anthropogenic influence. The high tritium contents would seem to be more problematic because of their consistent values over the total monitoring period of almost a year. However, high tritium occurs also in the deeper samples described below, and therefore a young origin to the sampled groundwaters may still be valid. The presence of such a young, weak brackish groundwater at this depth, suggests possible short circuiting/mixing from shallower levels (possibly facilitated by the long borehole section sampled at 43 m). This is supported by the hydraulic studies. The groundwater is therefore not considered representative for the sampled level. Allocated Category 5.

B2.1.2 KAV01 (420.00–425.00 m; mid. vertical elevation: –408.30 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					x
Drilling water (> 10%)					
Time series (adequate)					x
Time series (inadequate)					
Time series absent					
Suitable section length					x
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L 99Cl)					x
Major ions (complete)					x
Major ions (incomplete)					
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring section					
Hydraulic effects (short circuiting)					x?

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –0.4% to +2.63%.

Time Series: 1987-09-02 to 1987-09-23 (21 days). Adequate time series (6 samples) showing a progressive increase in salinity during the sampling period (350–616 mg/L Cl), supported by increases in the other major ions. Drilling water between 5–10% but increases with time (7.2–9.6%). Major ion data complete for two of the sampled occasions but general absence of TOC.

Isotopes: Incomplete isotopes; no ^{14}C. For the second last and only sample δ^{13}C records –20.4‰ PDB, tritium at 19 TU and δ^{18}O at –10.6‰ VSMOW.

Trace elements: Lack of data.

General: Na(Ca)-Cl(HCO_3) weak brackish groundwater similar to the preceding section but now showing a low, but increasing amount of Mg (18–29 mg/L) with time, together with a slightly more enriched δ^{18}O. These observations may indicate the appearance of a weak marine component.

Comment: Adequate time series with general coverage of major elements, but absence of trace elements and ^{14}C. Groundwater instability with time with an increase in all major ions may indicate a small increase in a marine component. In any case, this groundwater supports the preceding sample in that the presence of such a young, weak brackish groundwater at this depth indicates probable short circuiting/mixing. Furthermore, drilling water remains at significant levels. The groundwater is therefore not considered representative for the sampled level. Allocated Category 5.

B2.1.3 KAV01 (522.00–531.00 m; mid. vertical elevation: –512.18 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					x
Drilling water (> 10%)					
Time series (adequate)					x
Time series (inadequate)					
Time series absent					
Suitable section length					x
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring section					
Hydraulic effects (short circuiting)					x?

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –2.19% to +2.94%.

Time Series: 1987-08-04 to 1987-08-25 (21 days). Adequate time series (9 samples) showing a progressive increase in salinity during the sampling period (1,160–1,970 mg/L Cl), supported by increases in Na, Ca and SO_4, and a decrease in HCO_3; Mg ranges from 35–42 mg/L with a possible small increase with time. Drilling water is consistent varying between 7.8–11.0%. Major ion data are incomplete; sporadic for Li, Sr and DOC and TOC is absent.

Isotopes: Incomplete isotopes; no ^{14}C. The final and only sample records $\delta^{13}C$ at –20.4‰ PDB, tritium at 13 TU and $\delta^{18}O$ at –10.9‰ VSMOW.

Trace elements: Lack of data.

General: Na(Ca)-Cl(HCO_3) brackish groundwater similar to the preceding two sections; still young but now of greater salinity (~ 2,000 mg/L Cl), significantly higher Na, Ca and SO_4, lower HCO_3 and similar $\delta^{18}O$ content.

Comment: Adequate time series with general coverage of major elements, but absence of trace elements and ^{14}C. Groundwater instability with time with an increase in all major ions indicating an increasing component of deeper groundwater (including a small increased marine component) entering the sampled borehole section, compared with the preceding two sampled levels. Drilling water remains at high levels and once again short circuiting/mixing has probably played an important part. The groundwater is therefore not considered representative for the sampled level. Allocated Category 5.

B2.1.4 KAV01 (558.00–563.00 m; mid. vertical elevation: –546.14 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)				x	
Time series (adequate)				x	
Time series (inadequate)					
Time series absent					
Suitable section length				x	
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)				x	
Major ions (incomplete)					
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring section					
Hydraulic effects (short circuiting)				x?	

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –1.86% to +5.38%; initial groundwater sample at –33.98% (sample 1356) excluded.

Time Series: 1987-05-05 to 1987-06-03 (29 days). Adequate time series (18 samples) show an initial 15 day period of saline stability (~ 4,100 mg/L Cl) followed by a slight increase to 4,300 mg/L Cl for the remaining sampling time. Drilling water is consistently high ranging from 15.1–17.1% with no systematic change. Major ion data are complete but sporadically some samples lack one or more of Br, F, Si, Li, Sr and DOC (TOC is generally absent).

Isotopes: Incomplete isotopes; no ^{14}C. The final and only sample records δ^{13}C at –20.2‰ PDB, tritium at 8 TU and δ^{18}O at –11.7‰ VSMOW.

Trace elements: Lack of data.

General: Na(Ca)-Cl(SO$_4$ brackish groundwater.

Comment: Adequate time interval series in general with adequate coverage of major elements, but absence of trace elements and ^{14}C and retaining a very high drilling water content. Compared to the previous sections, this groundwater has a higher salinity but still brackish in type with a somewhat higher Mg (60–70 mg/L) and a slightly more depleted δ^{18}O value. The suspiciously constant chemistry during the first 15 days (and then for the final 3 days at slightly higher salinity) indicates a mixed homogeneous source and short circuiting is suspected. Despite this observation and the high drilling water content, the groundwater is more representative of this depth than the previously sampled sections. Allocated Category 4.

B2.1.5 KAV01 (635.00–743.60 m; mid. vertical elevation: –674.69 m

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)			x		
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)			x		
Time series (inadequate)					
Time series absent					
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)			x?		

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –1.13% to +1.46%; five samples are excluded (1339, 1340, 1346, 1348 and 1352) because > ±5%.

Time Series: 1987-03-25 to 1987-04-22 (28 days). Adequate time series (17 samples) showing overall saline stability during the complete sampling period (9,700–9,800 mg/L Cl), this is supported by the other major ions. Drilling water data largely absent apart from three samples measured close to the end of the sampling period which indicated < 1%. Major ion data mostly complete but sporadic for most ions; absent are Sr and TOC.

Isotopes: Incomplete isotopes; no carbon isotopes (lack of HCO_3 ~ 9 mg/L). Tritium below detection limit (< 3 TU at this time), and depleted $\delta^{18}O$ value at –12.8‰ VSMOW suggesting a weak cold climate component.

Trace elements: Lack of data.

General: Na(Ca)-Cl(SO_4) brackish non-marine type groundwater, when compared to the previous sections.

Comment: Adequate time interval series with adequate coverage of major elements, but absence of trace elements and no time series data for $\delta^{18}O$ or tritium. Furthermore, a long borehole section is involved (108.60 m) which, together with some short circuiting, may explain the homogeneity of the sampled groundwaters, although there is no evidence of short circuiting from shallower depths. In general, however, this groundwater is considered to be largely representative of the sampled depth, i.e. brackish non-marine in type with low Mg (~ 30 mg/L; although still possibly indicating a weak marine component) and an even more depleted $\delta^{18}O$ value than the preceding borehole section confirming an increasing cold climate signature. Second last sample is chosen because of isotopic data; absent major data can be extrapolated from the earlier time series. Allocated Category 3.

B2.2 Borehole KAV04

The main reason for drilling borehole KAV04 (1,004.0 m at –84.90° to the horizontal and cased to 100.0 m) was to gain geological information at depth of the northern part of the Simpevarp subarea and to facilitate further investigation (i.e. hydrogeology and hydrochemistry) at depth in the borehole. Drilling was carried out from 2003-10-06 to 2004-05-03.

B2.2.1 KAV04 (0–100.20 m; mid. vertical elevation: –39.56 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)				x	
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)				x	
Time series absent					
Suitable section length					
Sampling during drilling				x	
Sampling using PLU hydraulic testing equipment				x	
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring section					
Hydraulic effects (short circuiting)				x?	

Drilling Water: Two water sources were used during the drilling of KAV04. Initially the percussion drilled borehole HLX10 was used and the water was brought in by truck. In the period between January 18 and 28, 2004, corresponding to drilling between 260 and 280 metres, water was intermittently used from both HLX10 and HSH03 because the hoses from HSH03 were frequently frozen. After January 28, 2004 i.e. below 280 metres drilled length, water was taken from HSH03.

HLX10 (0–85 m; mid. vertical elevation: –27.86 m). There is no documented sample from the time of drilling borehole KLX02 from 1992-08-15 to 1992-09-05; in the Extended L.2.3 dataset one sample is documented from 2003-03-12 and used here. Na-HCO$_3$ type groundwater with low chloride (6.3 mg/L) and with enriched δ^{18}O at –10.9‰ VSMOW and δ^{2}H at –78.8‰ VSMOW; tritium at 7.2 TU, δ^{13}C at –17.45‰ PDB and ^{14}C at 55.73 pmC.

HSH03 (0–103 m; mid. vertical elevation: –48.11 m). Sample considered closest to being representative (sampled 2002-08-22, Extended L.2.3 database) is documented prior to the drilling of the borehole from 2003-10-06 to 2004-05-03. Na-HCO$_3$(SO$_4$,Cl) type groundwater with low chloride (55.1 mg/L) and with enriched δ^{18}O at –10.7‰ VSMOW and δ^{2}H at –76.1‰ VSMOW; tritium at 10 TU, δ^{13}C at –17.80‰ PDB and ^{14}C at 61.00 pmC.

Charge Balance: Sicada measured values at –5.83% to +1.75%.

Time Series: 2003-10-09 to 2003-10-21 (12 days). Only one sample taken using PLU hydraulic testing equipment during drilling. Inadequate time series (2 samples) showing a small decrease in salinity (37.4–25.7 mg/L Cl). Drilling water < 1% with a small decrease during the sampling period (0.13–0.06%). Major ion data incomplete; no Fe(tot), Fe^{2+}, S^{2-} or TOC.

Isotopes: Complete isotopes (last sample); ^{14}C at 46.25 pmc, δ^{13}C at –16.53‰ PDB. Tritium at 2.8 TU and δ^{18}O at –10.9‰ VSMOW.

Trace elements: Lack of data.

General: Na-HCO$_3$ fresh meteoric recharge groundwater.

Comment: Groundwater may be quite representative of the sampled depth; however, it originates from a 0–100.20 m borehole length where mixing/short circuiting has probably occurred. This feature, together with a general absence of time series and trace elements, and incomplete major ions, point to a Category 4 for the final sample.

B2.2.2 KAV04 (47.60–50.60 m; mid. vertical elevation: –38.56 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					x
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					
Sampling during drilling					x
Sampling using PLU hydraulic testing equipment					x
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring section					
Hydraulic effects (short circuiting)					x?

Drilling Water: Two water sources were used during the drilling of KAV04. Initially the percussion drilled borehole HLX10 was used and the water was brought in by truck. In the period between January 18 and 28, corresponding to drilling between 260 and 280 metres, water was intermittently used from both HLX10 and HSH03 because the hoses from HSH03 were frequently frozen. After January 28, i.e. below 280 metres drilled length, water was taken from HSH03.

HLX10 (0–85 m; mid. vertical elevation: –27.86 m). There is no documented sample from the time of drilling borehole KLX02 from 1992-08-15 to 1992-09-05; in the Extended L.2.3 dataset one sample is documented from 2003-03-12 and used here. Na-HCO$_3$ type groundwater with low chloride (6.3 mg/L) and with enriched δ^{18}O at –10.9‰ VSMOW and δ^{2}H at –78.8‰ VSMOW; tritium at 7.2 TU, δ^{13}C at –17.45‰ PDB and ^{14}C at 55.73 pmC.

HSH03 (0–103 m; mid. vertical elevation: –48.11 m). Sample considered closest to being representative (sampled 2002-08-22, Extended L.2.3 database) is documented prior to the drilling of the borehole from 2003-10-06 to 2004-05-03. Na-HCO$_3$(SO$_4$,Cl) type groundwater with low chloride (55.1 mg/L) and with enriched δ^{18}O at –10.7‰ VSMOW and δ^{2}H at –76.1‰ VSMOW; tritium at 10 TU, δ^{13}C at –17.80‰ PDB and ^{14}C at 61.00 pmC.

Charge Balance: Sicada measured value at –8.26% (permitted to ±10%).

Time Series: Only one sample taken using PLU hydraulic testing equipment during drilling in 2003-10-09. Time series absent. Groundwater is fresh (22.6 mg/L Cl) with a drilling water content of 0.54%. Major ions incomplete; no F, Fe(tot), Fe(II), S^{2-} or TOC/DOC.

Isotopes: Lack of data.

Trace elements: Lack of data.

General: Na-HCO_3 fresh groundwater.

Comment: Fresh groundwater in all probability representative of the sampled level. However, absence of time series, incomplete major ion data, and a lack of isotope and trace element data, points to a Category 5 sample.

KAV04: Tube samples sampled every 50 m from 00.00–945.00 m (2004-06-08) are considered unrepresentative and allocated Category 5.

Note: *Although open hole tube samples are generally judged to be Category 5, this sampled series from borehole KAV04 provides a good example of the qualitative use of tube sample data. The data series gives a clear idea as to the systematic change in hydrochemistry with depth (increase in salinity (Cl), Ca and* SO_4*), decrease in* HCO_3 *and Mg etc, and depletion of* $\delta^{18}O$*. This helps, therefore, to put the KAV01 samples into a better perspective, emphasising the short circuiting which has influenced the upper ~ 500 m of the borehole.*

Laxemar data

C1 Percussion boreholes

C1.1 HLX01 (50.00–100.00 m; mid. vertical elevation: –56.19 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)				x	
Section without flow log (0–100 m)					
Section without flow log (0–200 m)					
Time series/monitoring				x	
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at +2.74% to +6.66% (permitted to ±10%).

Time Series: 1987-10-23 to 1987-10-25 (3 days) using the PLU hydraulic testing equipment. Inadequate time series (3 samples). Excluding the first sample, the remaining 2 samples stabilise around 41 mg/L Cl and the other major ions show a small increase. Incomplete major ions; no Br, Si, Mn, Li, Sr, S^{2-}, Fe^{2+} and TOC.

Isotopes: Incomplete isotopes; no carbon isotopes. Tritium high, decreasing from 34–17 TU and $\delta^{18}O$ at –10.9‰ VSMOW.

Trace elements: Lack of data.

General: Na-HCO_3 fresh, meteoric recharge type groundwater.

Comment: Limited time series, lack of major elements and carbon isotopes, and absence of trace element data, coupled with a long 50 m borehole length (probably facilitating mixing/short circuiting). However, such a groundwater composition is expected at such shallow depths. Allocated Category 4 to the final sample.

C1.2 HLX03 (25.00–100.00 m; mid. vertical elevation: –46.69 m)

Percussion Borehole					
Category	**1**	**2**	**3**	**4**	**5**
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)					
Section without flow log (0–100 m)				x	
Section without flow log (0–200 m)					
Time series/monitoring				x	
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at +3.59 to +3.69%.

Time Series: 1987-11-05 to 1987-11-06 (2 days) using the PLU hydraulic testing equipment. Inadequate time series (2 samples) which show a small decrease in salinity (11.0–5.8 mg/L Cl). Incomplete major ions; no Br, F, Si, Mn, Li, Sr, S^{2-}, Fe^{2+} and TOC.

Isotopes: Incomplete isotopes; no carbon isotopes. Tritium is high, increasing from 25–34 TU and $\delta^{18}O$ at –10.90 to –19.80‰ VSMOW.

Trace elements: Lack of data.

General: Na-HCO_3 fresh, meteoric recharge type groundwater.

Comment: Limited time series, lack of some major elements and carbon isotopes, absence of trace element data, and a long (70 m) borehole section (possibly facilitating mixing/short circuiting). However, such a groundwater composition is expected at such shallow depths. Allocated Category 4 to the final sample.

C1.3 HLX06 (45.00–100–00 m; mid. vertical elevation: –46.42 m)

Percussion Borehole					
Category	**1**	**2**	**3**	**4**	**5**
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)					
Section without flow log (0–100 m)				x	
Section without flow log (0–200 m)					
Time series/monitoring				x	
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –0.52% to +2.71%.

Time Series: 1987-11-01 to 1987-11-03 (3 days) using the PLU hydraulic testing equipment. Inadequate time series (2 samples) showing a small increase in salinity (5.7–12.1 mg/L Cl) together with small increases in Na, HCO_3 and SO_4, and decreases in Ca and Mg. Incomplete major ions; no Br, F, Si, Mn, Li, Sr, S^{2-}, Fe^{2+} and TOC.

Isotopes: Incomplete isotopes; no carbon isotopes. Tritium is high at 17 TU for both samples and $\delta^{18}O$ at –10.6‰ VSMOW.

Trace elements: Lack of data.

General: Na-HCO_3 fresh, meteoric recharge type groundwater.

Comment: Inadequate time series, lack of some major elements and carbon isotopes, absence of trace element data, and long borehole section (55 m possibly facilitating mixing/short circuiting). However, such a groundwater composition is expected at such shallow depths. Allocated Category 4 to the final sample.

C1.4 HLX07 (20.00–100.00 m; mid. vertical elevation: –44.76 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					x
Section without flow log (0–200 m)					
Time series/monitoring					x
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –3.3% to +1.44%

Time Series: 1987-11-04 to 1987-11-05 (2 days) using the PLU hydraulic testing equipment. Inadequate time series (2 samples) showing an increase in salinity (215–440 mg/L Cl) together with increases in all the remaining major ions. Incomplete major ions; no Br, F, Si, Mn, Li, Sr, S^{2-}, Fe^{2+} and TOC.

Isotopes: Incomplete isotopes; no carbon isotopes. Tritium decreases from 25–8.4 TU and $\delta^{18}O$ at –10.8 to –10.4‰ VSMOW, both indicating modern meteoric recharge conditions.

Trace elements: Lack of data.

General: Na–$HCO_3(Cl,SO_4)$ brackish groundwater.

Comment: Inadequate time series, lack of some major elements and carbon isotopes, absence of trace element data, and long borehole section (80 m) possibly facilitating mixing/short circuiting. Together with the marked change in chemistry between the two samples, a Category 5 has been allocated to both samples.

C1.5 HLX10 (00–85.00 m; mid. vertical elevation: –27.86 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					x
Section without flow log (0–200 m)					
Time series/monitoring					
Time series absent					x
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Charge Balance: Sicada measured value is +0.66%.

Time Series: 2003-03-12; absence of time series (1 sample). Salinity at 6.3 mg/L Cl; drilling water < 1% (0.02%). Incomplete major ions; no Fe(tot), Fe^{2+}, S^{2-} and DOC.

Isotopes: Complete isotopes; $\delta^{13}C$ at –17.45‰ PDB, ^{14}C at 53.73 pmC, tritium at 7.2 TU and $\delta^{18}O$ at –10.9‰ VSMOW.

Trace elements: Lack of data.

General: Na-HCO_3 fresh, meteoric recharge type groundwater.

Comment: No time series, lack of some major elements, absence of trace element data, and a long borehole section (85 m) which may facilitate mixing/short circuiting. Allocated Category 5.

C1.6 HLX10 (03–85.00 m; mid. vertical elevation: –29.25 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)					
Section without flow log (0–100 m)			x		
Section without flow log (0–200 m)					
Time series/monitoring					
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)			x?		

Charge Balance: Measured Sicada values at +0.44% to –1.57%.

Time Series: 2005-02-01 to 2005-10-28 (two occasions ~ 9 months apart). Inadequate time series (2 samples) but saline stability indicated (29.1–31.9 mg/L Cl), supported by the remaining major ions. Some drilling water (0.24%) recorded for the first sampled occasion. Incomplete major ions; no Fe(tot), Fe^{2+}, S^{2-} and DOC.

Isotopes: Complete isotopes; $\delta^{13}C$ at –16.43 to –16.12‰ PDB, ^{14}C at 51.72–52.73 pmC, tritium at 5.2–5.7 TU, and $\delta^{18}O$ at –10.9 to –10.8‰ VSMOW.

Trace elements: Lack of data.

General: $Na\text{-}HCO_3(SO_4,Cl)$ fresh, meteoric recharge type groundwater.

Comment: Inadequate time series, lack of some major ions, absence of trace element data, and long borehole section (82 m) possibly facilitating mixing/short circuiting. However, because of the long term stability of the near-surface groundwater chemistry, and that most of the major ion data and complete isotope data are present, a Category 3 has been allocated to the last sampled groundwater.

C1.7 HLX14 (11.90–115.90 m; mid. vertical elevation: –42.17 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log			x		
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					
Section without flow log (0–200 m)					
Time series/monitoring			x		
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)			x		
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)			?		

Charge Balance: Measured Sicada values at –1.91% to –2.75%.

Time Series: 2004-05-07 to 2006-11-04 (two occasions, 2.5 years apart) showing a marked increase in salinity (69.70–357.00 mg/L Cl) supported by the remaining ions apart from a decrease in HCO_3 (302–223 mg/L). Drilling water is reported as 0.05% for the 2006 sample. Incomplete major ions; no Fe(tot), Fe^{2+}, S^{2-} and DOC.

Isotopes: Complete isotopes; $\delta^{13}C$ at –18.50 to –17.20‰ PDB, ^{14}C at 54.70–49.70 pmC, tritium decreases from 3.8 TU in the initial sample to around 2.5 TU for the second one, and $\delta^{18}O$ values are constant at –11.2‰ VSMOW.

Trace elements: Lack of data.

General: $Na\text{-}HCO_3(Cl,SO_4)$ brackish, meteoric recharge type groundwater.

Comment: Inadequate time series, instability, lack of some major ions, absence of trace element data and long borehole section (110 m) possibly facilitating mixing/short circuiting. However, based on the flow logging (most groundwater input to the borehole is at 110.0–110.5 m (–85.18 m vertical elevation)), the second sample (2006) has been chosen as being more representative of a slightly deeper groundwater than indicated by the first sample. Furthermore, < 1% drilling water is indicated and most of the major ion data and complete isotope data are present. Allocated Category 3.

C1.8 HLX20 (9.10–202.20 m; mid. vertical elevation: –80.67 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					
Section without flow log (0–200 m)					x
Time series/monitoring					
Time series absent					x
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Charge Balance: Measured Sicada value at –1.94%.

Time Series: 2004-06-24; absence of time series (1 sample). Salinity at 29.4 mg/L Cl. Incomplete major ions; no Fe(tot), Fe^{2+}, S^{2-} and DOC.

Isotopes: Complete isotopes; $\delta^{13}C$ at –17.01‰ PDB, ^{14}C at 41.68 pmC, tritium under detection (< 0.8 TU), and $\delta^{18}O$ at –11.3‰ VSMOW.

Trace elements: Lack of data.

General: Na-HCO_3(SO_4,Cl) fresh meteoric groundwater.

Comment: No time series, lack of some major elements, absence of trace element data, and a long borehole section (193.10 m) possibly facilitating mixing/short circuiting, indicate a Category 5 sample.

C1.9 HLX20 (71.00–80.00 m; mid. vertical elevation: –54.46 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length			x		
Section with flow log					
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					
Section without flow log (0–200 m)					
Time series/monitoring					
Time series absent			x		
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)			x		
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Charge Balance: Measured Sicada value at –2.44%.

Time Series: 2007-06-18; absence of time series (1 sample). Fresh groundwater (50.2 mg/L Cl). Incomplete major ions; no Fe(tot), Fe^{2+}, S^{2-} and DOC.

Isotopes: Complete isotopes; $\delta^{13}C$ at –16.80‰ PDB, ^{14}C at 41.50 pmC, tritium at 1 TU, and $\delta^{18}O$ at –11.5‰ VSMOW.

Trace elements: Good coverage.

General: Na-HCO_3(Cl,SO_4) fresh, meteoric recharge type groundwater.

Comment: No time series, but when compared to the previous sample there is a reasonable similarity in composition despite the time interval of three years and the considerable difference in sampled borehole length. In general terms, this groundwater is considered typical of that expected at this shallow depth. Allocated Category 3.

C1.10 HLX21 (0–150.30 m; mid. vertical elevation: –50.82 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log					x
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					
Section without flow log (0–200 m)					
Time series/monitoring					
Time series absent					x
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Charge Balance: Measured Sicada value at –0.27%.

Time Series: 2006-05-18; absence of time series (1 sample). Major flow log input at 86.50–87.00 m (–59.94 m vertical elevation).Fresh groundwater (90.6 mg/L Cl). Incomplete major ions; no Fe(tot), Fe^{2+}, S^{2-} and DOC.

Isotopes: Lack of data.

Trace elements: Lack of data.

General: Na–HCO_3(SO_4, Cl) fresh, meteoric recharge type groundwater.

Comment: No time series, lack of some major elements, absence of isotope and trace element data, and a long borehole section (150.30 m) possibly facilitating mixing/short circuiting. Allocated Category 5.

C1.11 HLX21 (9.03–150.30 m; mid. vertical elevation: –54.37 m)

Percussion Borehole Category	**1**	**2**	**3**	**4**	**5**
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					
Section without flow log (0–200 m)				x	
Time series/monitoring				x	
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)				x	
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Charge Balance: Measured Sicada values at +4.56% to +2.65%.

Time Series: 2005-08-15 to 2005-08-19 (5 days). Inadequate time series (2 samples) showing a decrease in salinity (112–72.5 mg/L Cl) supported by decreases in Na, K, Ca, Mg, HCO_3 and SO_4. Incomplete major ions; no Fe (tot), Fe^{2+}, S^{2-} and TOC/DOC (in addition no Br in the first sampled occasion).

Isotopes: Complete isotopes; $\delta^{13}C$ at –14.92 to –13.36‰ PDB, ^{14}C at 42.07–46.44 pmC, tritium at 3.2–5.2 TU, and $\delta^{18}O$ values at –10.7 to 10.6‰ VSMOW.

Trace elements: Lack of data.

General: Na-HCO_3(Cl, SO_4) fresh, meteoric recharge type groundwater.

Comment: Inadequate time series and long sampling section, possibly facilitating mixing/short circuiting. Allocated Category 4.

C1.12 HLX22 (0–163.20 m; mid. vertical elevation: –57.00 m)

Percussion Borehole Category	**1**	**2**	**3**	**4**	**5**
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					
Section without flow log (0–200 m)				x	
Time series/monitoring					
Time series absent				x	
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)				x	
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Charge Balance: Measured Sicada value at –1.69%.

Time Series: 2004-09-17; absence of time series (1 sample). Fresh groundwater (23 mg/L Cl). Incomplete major ions; no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Complete isotopes; δ^{13}C at –15.19‰ PDB, ^{14}C at 49.51 pmC, tritium at 6.4 TU and a δ^{18}O value at –11.3‰ VSMOW.

Trace elements: Lack of data.

General: Na-HCO$_3$(SO$_4$) fresh, meteoric recharge type groundwater.

Comment: No time series, lack of some major elements, absence of trace element data, and a long borehole section (163.20 m) possibly facilitating mixing/short circuiting. However, because of good major ion and isotope data, and in general terms the groundwater is considered typical of that expected at this shallow depth. Allocated Category 4.

C1.13 HLX23 (0–160.20 m; mid. vertical elevation: –51.94 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					
Section without flow log (0–200 m)				x	
Time series/monitoring				x	
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)				x	
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)				x	

Charge Balance: Measured Sicada values at –1.17% to –3.09%.

Time Series: 2005-06-28 to 2005-07-01 (on two occasions 4 days apart). Inadequate time series (2 samples) showing only a very small range in salinity (51.5–56.9 mg/L Cl) and also the other major ions. Incomplete major ions; no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Complete isotopes; δ^{13}C at –16.81 to –16.39‰ PDB, ^{14}C at 54.54–57.91 pmC, tritium at 7–5.2 TU, and δ^{18}O values at –11.0% to 11.30‰ VSMOW.

Trace elements: Lack of data.

General: Na-HCO$_3$(SO$_4$) fresh, meteoric recharge type groundwater.

Comment: Inadequate time series, lack of some major elements, absence of trace element data, and a long borehole section (160.20 m) possibly facilitating mixing/short circuiting. However, because of adequate major ion and good isotope data, and in general terms the groundwater is considered typical of that expected at this shallow depth, a Category 4 is allocated to the most recent sample collected.

C1.14 HLX24 (0–175.20 m; mid. vertical elevation: –59.62 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					
Section without flow log (0–200 m)				x	
Time series/monitoring					
Time series absent				x	
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)				x	
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Charge Balance: Measured Sicada value at +1.87%.

Time Series: 2004-09-10; absence of time series (1 sample). Fresh groundwater (15.1 mg/L Cl). Incomplete major ions; no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Complete isotopes; $\delta^{13}C$ at –12.54‰ PDB, ^{14}C at 77.87 pmC, tritium at 10.5 TU and $\delta^{18}O$ at –10.8‰ VSMOW.

Trace elements: Lack of data.

General: $Na\text{-}HCO_3$ fresh, meteoric recharge type groundwater.

Comment: No time series, lack of some major elements, absence of trace element data, and a long borehole section (175.20 m) possibly facilitating mixing/short circuiting. However, because of good major ion and isotope data, and in general terms the groundwater is considered typical of that expected at this shallow depth. Allocated Category 4.

C1.15 HLX28 (6.03–154.20 m; mid. vertical elevation: –52.67 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log			x		
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					
Section without flow log (0–200 m)					
Time series/monitoring			x		
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)			x		
Environmental isotopes (incomplete)					
Monitoring borehole section			x		
Hydraulic effects (short circuiting)			x?		

Charge Balance: Measured Sicada values at –2.23% to +0.92%.

Time Series: 2005-04-12 to 2006-03-10 (11 months). Major flow log input at 78.00–79.50 m (–52.67 m vertical elevation). Monitoring borehole section (3 samples) showing a small increase in salinity (23.0–39.3 mg/L Cl) supported by small increases in Ca, Mg and SO_4 and a decrease in HCO_3. Drilling water recorded in 2006 is 0.98% indicating some type of contamination. Incomplete major ions; no Fe(tot), Fe^{2+}, S^{2-} and DOC.

Isotopes: Complete isotopes for the 2006 sample; $\delta^{13}C$ at –16.15‰ PDB, ^{14}C at 46.91 pmC, tritium at 1 TU, and $\delta^{18}O$ at –10.9‰ VSMOW.

Trace elements: Lack of data.

General: Na-$HCO_3(SO_4)$ fresh meteoric groundwater.

Comment: Inadequate time series for isotopes, lack of some major elements, absence of trace element data, and a long borehole section (148.17 m) possibly facilitating mixing/short circuiting. However, because of good major ion and on the first sampling occasion good isotope data, together with reasonably good stability over a 11 month period, in general terms the groundwater is considered typical of that expected at this shallow depth (major groundwater input based on the flow log is from about at 78.00–79.50 m (–52.67 m vertical elevation)). A Category 3 is allocated to the first sample collected in 2005-04-12, i.e. prior to subsequent small, but progressive changes in composition with time.

C1.16 HLX30 (0–163.40 m; mid. vertical elevation: –60.04 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					
Section without flow log (0–200 m)			x		
Time series/monitoring			x		
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)			x		
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)			x?		

Charge Balance: Measured Sicada values at +1.69% to +2.68%.

Time Series: 2005-06-09 to 2005-09-05 (sampling interval of ~ 3 months). Inadequate time series (2 samples) showing an increase in salinity (428–520 mg/L Cl) supported by small increases in Na, Ca, K. Mg and SO_4 and a decrease in HCO_3. Incomplete major ions; no Br, Fe(tot), Fe^{2+}, S^{2-} and DOC.

Isotopes: Complete isotopes; $\delta^{13}C$ at –14.99 to –13.44‰ PDB, ^{14}C at 34.11–38.16–pmC, tritium under detection (< 0.8 TU), and $\delta^{18}O$ values at –13.5 to –13.1‰ VSMOW indicate a significant cold climate signature.

Trace elements: Lack of data.

General: Na-Cl(HCO_3,SO_4) brackish glacial groundwater.

Comment: Inadequate time series, lack of some major elements, absence of trace element data, and a long borehole section (163.40 m) possibly facilitating mixing/short circuiting. However, because of good major ion and good isotope data, together with reasonably good stability over the 3 month period, in general terms the groundwater is considered typical of that expected at shallow to intermediate depth. A Category 3 is allocated to the most recent sample.

C1.17 HLX33 (9.03–202.10 m; mid. vertical elevation: –84.94 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log				x	
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					
Section without flow log (0–200 m)					
Time series/monitoring					
Time series absent				x	
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)				?	

Charge Balance: Measured Sicada value at +0.03%.

Time Series: 2006-06-29; absence of time series (1 sample). Flow log indicates major groundwater input at 111.00–111.50 m (–84.94 m vertical elevation). Fresh groundwater (128 mg/L Cl). Incomplete major ions; no Fe(tot), Fe^{2+}, S^{2-} and DOC.

Isotopes: Complete isotopes; no carbon isotopes. Tritium at 3.6TU and $\delta^{18}O$ at –10.7‰ V-SMOW.

Trace elements: Lack of data.

General: Na-HCO_3(Cl,SO_4) fresh, meteoric recharge type groundwater.

Comment: No time series, lack of some major elements, incomplete isotope data, an absence of trace element data, and a long borehole section (193.07 m) possibly facilitating mixing/short circuiting. However, because of good major ion and isotope data, and in general terms the groundwater is considered typical of that expected in the upper bedrock and where most input based on the flow log is, a Category 4 is allocated.

C1.18 HLX34 (0–151.80 m; mid. vertical elevation: –50.17 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					
Section without flow log (0–200 m)				x	
Time series/monitoring				x	
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Charge Balance: Measured Sicada values at –1.62% to –0.54%.

Time Series: 2005-06-16 (1 day). Inadequate time series (2 samples) showing a little change in salinity (45.1–44.4 mg/L Cl) supported by the remaining major ions. Incomplete major ions; no Br, Fe(tot), Fe^{2+}, S^{2-} and DOC.

Isotopes: Complete isotopes; δ^{13}C at –16.51 to –16.50‰ PDB, ^{14}C at 42.46–42.55 pmC, tritium under detection (< 0.8 TU) and δ^{18}O values at –11.2‰ VSMOW.

Trace elements: Lack of data.

General: Na-HCO$_3$(SO$_4$,Cl) fresh, meteoric recharge type.groundwater.

Comment: Inadequate time series, lack of some major elements, absence of trace element data, and a long borehole section (151.80 m) possibly facilitating mixing/short circuiting. However, because of good major ion and isotope data, and in general terms the groundwater is considered typical of that expected at shallow to intermediate depth, a Category 4 is allocated to the last sample collected.

C1.19 HLX35 (6.03–151.80 m; mid. vertical elevation: –89.75 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log			x		
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					
Section without flow log (0–200 m)					
Time series/monitoring			x		
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)			?		

Charge Balance: Measured Sicada values at –0.43% to +0.80%.

Time Series: 2006-11-16 to 2006-11-18 (3 days). Flow log indicates major groundwater input at 123.00–134.00 m (–89.55 m vertical elevation). Inadequate time series (2 samples) showing an increase in salinity (154–203 mg/L Cl) supported by small increases in all remaining major ions. Incomplete major ions; no Br, Fe(tot), Fe^{2+}, S^{2-} and DOC.

Isotopes: Complete isotopes; δ^{13}C at –16.43 to –16.14‰ PDB, ^{14}C at 41.60–48.07 pmC, tritium at 1.5–2.2 TU, and δ^{18}O values at –11.3 to –11.4‰ VSMOW.

Trace elements: Lack of data.

General: Na-HCO$_3$(Cl,SO$_4$) fresh, meteoric recharge groundwater.

Comment: Inadequate time series, lack of some major elements, absence of trace element data, and a long borehole section (145.77 m) possibly facilitating mixing/short circuiting. However, because of good major ion and isotope data, and in general terms the groundwater is considered typical of that expected in the upper bedrock where most input based on the flow log is known, a Category 3 is allocated.

C1.20 HLX37 (12.03–199.80 m; mid. vertical elevation: –69.00 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log				x	
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					
Section without flow log (0–200 m)					
Time series/monitoring				x	
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)				x	
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Charge Balance: Measured Sicada values are at –0.51 to +1.61%.

Time Series: 2005-10-18 to 2005-11-10 (23 days). Flow log indicates major groundwater input at 97.00–100.50 m (–69.00 m vertical elevation). Inadequate time series (3 samples) showing a marked increase in salinity (12.8–109 mg/L Cl) supported by small increases in all remaining major ions apart from a decrease in HCO$_3$. Incomplete major ions; no Br, Fe(tot), Fe^{2+}, S^{2-} and DOC (only one TOC value).

Isotopes: Complete isotopes; δ^{13}C at –16.02 to –15.41 PDB, ^{14}C at 40.54–44.13 pmC, tritium at 1.3–2.3TU, and δ^{18}O values at –11.0 to –11.3‰ V-SMOW.

Trace elements: Lack of data.

General: Na-HCO$_3$-Cl(SO$_4$) fresh, meteoric recharge groundwater.

Comment: Inadequate time series, instability, lack of some major elements, absence of trace element data, and a long borehole section (145.77 m) possibly facilitating mixing/short circuiting. However, because of good major ion and isotope data, and in general terms the groundwater is considered typical of that expected in the upper bedrock where most input based on the flow log is known, a Category 4 is allocated to the intermediate sample collected.

C1.21 HLX38 (15.02–199.50 m; mid. vertical elevation: –28.73 m)

Percussion Borehole					
Category	**1**	**2**	**3**	**4**	**5**
Short restricted section length					
Section with flow log				x	
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					
Section without flow log (0–200 m)					
Time series/monitoring					
Time series absent				x	
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Charge Balance: Measured Sicada value at +0.23%.

Time Series: 2006-05-22; absence of time series (1 sample). Flow log indicates major groundwater input at 29.50–65.50 m (–14.17 m to –43.30 m vertical elevation). Brackish groundwater (839 mg/L Cl). Incomplete major ions; no Fe(tot), Fe^{2+}, S^{2-} and DOC.

Isotopes: Complete isotopes; $\delta^{13}C$ at –14.78‰ PDB, ^{14}C at 51.05 pmC, tritium at 2.8 TU, and $\delta^{18}O$ at –11.9‰ VSMOW.

Trace elements: Lack of data.

General: Na(Ca)-Cl(HCO_3,SO_4) brackish meteoric groundwater.

Comment: No time series, lack of some major elements, an absence of trace element data, and a long borehole section (184.48 m) possibly facilitating mixing/short circuiting. However, because of good major ion and isotope data, and in general terms the groundwater is considered typical of that expected in the shallow bedrock, where most input based on the flow log is known, a Category 4 is allocated.

C1.22 HLX39 (6.02–199.30 m; mid. vertical elevation: –137.87 m)

Percussion Borehole					
Category	**1**	**2**	**3**	**4**	**5**
Short restricted section length					
Section with flow log				x	
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					
Section without flow log (0–200 m)					
Time series/monitoring					
Time series absent				x	
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)				x	
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Charge Balance: Measured Sicada value at +1.43%.

Time Series: 2006-05-22; absence of time series (1 sample). Flow log indicates major groundwater input at 191.00–192.50 m (–137.87 m vertical elevation). Fresh groundwater (26.4 mg/L Cl). Incomplete major ions; no Fe(tot), Fe^{2+}, S^{2-} and DOC.

Isotopes: Complete isotopes; $\delta^{13}C$ at –17.40‰ PDB, ^{14}C at 63.30 pmC, tritium at 6.2 TU and $\delta^{18}O$ at –11.2‰ VSMOW.

Trace elements: Lack of data.

General: Na(Ca)-HCO_3 fresh, meteoric recharge type groundwater.

Comment: No time series, lack of some major elements, an absence of trace element data, and a long borehole section (184.48 m) possibly facilitating mixing/short circuiting. However, because of adequate major ion and isotope data, and in general terms the groundwater is considered typical of the upper bedrock levels where most input based on the flow log is known, a Category 4 is allocated.

C2 Cored boreholes

C2.1 Description of Borehole KLX01

Borehole KLX01 was the first deep borehole to be drilled at the Laxemar site. In common with borehole KAV01, it was drilled prior to the site characterisation of the Laxemar-Simpevarp area and upgraded so it could be integrated in the Oskarshamn site investigation database. It was therefore drilled in two phases: a) to 702.10 m from 1987-12-05 to 1988-02-05, and b) from 702.10 to 1,077.99 m from 1990-05-07 to 1990-08-04, and inclined at –85.30° to the horizontal. The vertical depth is 1,076.12 m and the borehole is cased to 101.30 m borehole length. The borehole was used to obtain an initial impression of the bedrock at the Laxemar site that would help to further plan the hydrochemical investigations.

Differential Flow Log: The differential downhole flow log measurement technique was not available following drilling in 1988, but hydraulic injection tests to 700 m reveal a range of hydraulic conductivity from 10^{-10}–10^{-5} ms^{-1} along the borehole length with the most transmissive section extending from 101 m (extent of the casing) to approximately 470 m. Groundwater samples from 272–277 m and 456–461 m are representative for this transmissive section. At greater depths to 700 m hydraulic conductivities are somewhat lower, averaging at about 10^{-9} ms^{-1} with the exception of 650–700 m where values of 10^{-7}–10^{-6} ms^{-1} have been measured; this represents one of the groundwater sampling locations at 680.00–702.11 m. Groundwaters were taken also at greater depths, 910–921 m and 999–1,078 m respectively, with the latter corresponding to a significant fracture zone.

The variations in transmissivity relate to a series of intermediate to steeply dipping fracture zones that intersect the borehole between about 400–900 m vertical depth. These may facilitate short circuiting during sampling.

Electrical Conductivity log: No downhole electrical conductivity or hydrochemical logging (i.e. tube sampling) has been carried out.

Hydrochemical Logging: No hydrochemical borehole logging of KLX01 has been carried out.

References: SKB P-09-01, and R-06-01 and R-06-70 where earlier documentation of groundwater quality is given.

C2.1.1 KLX01 (171.00–190.00 m; mid. vertical elevation: –163.26 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)				x	
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)				x	
Time series absent					
Suitable section length				x	
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)				x	
Major ions (incomplete)					
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section				x	
Hydraulic effects (short circuiting)				x?	

Drilling Water: HLX05 (19.00–20.00 m). There is no documented sample from the time of drilling borehole KLX01 (i.e. first phase to 703.00 m in 1988 and second phase to 1,077. 99 m in 1990); in the Extended L.2.3 dataset one sample (Experiment Water) is documented from 2003-03-12 and used here. Na-HCO_3 type groundwater with low chloride (5.4 mg/L), enriched $\delta^{18}O$ at –9.7‰ VSMOW and δ^2H at –74.4‰ VSMOW; no tritium or carbon isotope data are available.

Charge Balance: Measured Sicada values at –1.49% to +0.32%.

Time Series: Monitoring section sampled on two occasions (2006-07-05 and 2006-10-31) of a fresh groundwater showing stability (110–122 mg/L Cl) over the approximately 4 month period, although more time series would have been desired. Drilling water < 1%. Major ions complete.

Trace elements: Good coverage.

Isotopes: Incomplete; no ^{14}C; $\delta^{13}C$ at –15.56‰ PDB, tritium at 3.8 TU and $\delta^{18}O$ at –10.6‰ VSMOW.

General: Na(Ca)-HCO_3(Cl,SO_4) fresh groundwater of shallow bedrock origin with a modern component indicated by the presence of tritium.

Comment: Stable groundwater with no drilling water component which is to be expected as this sampling took place some 18 years after drilling. Hydraulic tracer tests were carried out from 2005-11-29 to 2005-12-07 using uranine in section 171.00–190.00 m, i.e. prior to the groundwater sampling. However, these tests do not appear to have influenced the amount of 'drilling water' that would have resulted from any misinterpretation of enhanced uranine (cf section 3.1.1). Perhaps at these shallow depths, any effect has been flushed out of the system during the time gap of about 8 months. Furthermore, tracer tests were carried out at deeper levels (see next description below) and these also have had no effect. An additional problem is how representative are the data considering that sampling within the monitoring programme is carried out rapidly compared to the CCC protocol. For example, the higher pump rates used during monitoring may lead to short circuiting thus contributing to the overall uncertainty. Allocated Category 4.

C2.1.2 KLX01 (272.00–277.00 m; mid. vertical elevation: –257.06 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)			x		
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)			x		
Time series absent					
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HLX05 (19.00–20.00 m). There is no documented sample from the time of drilling borehole KLX01 (i.e. first phase to 703.00 m in 1988 and second phase to 1,077. 99 m in 1990); in the Extended L.2.3 dataset one sample (Experiment Water) is documented from 2003-03-12 and used here. Na-HCO$_3$ type groundwater with low chloride (5.4 mg/L) with enriched δ^{18}O at –9.7‰ VSMOW and δ^{2}H at –74.4‰ VSMOW; no tritium or carbon isotope data are available.

Charge Balance: No measured Sicada values are given but modelled PHREEQC value at –0.37%.

Time Series: 1988-11-25 to 1988-12-09 (15 days); adequate time series showing instability during the initial 7 days (1,640–2,020 mg/L Cl) followed by reasonable stability to the end of the sampling period (2,020–2,070 mg/L Cl); this is supported by the remaining major ions. During the sampling period the drilling water remained constant between 4.4–4.8%. Major ions almost complete (no TOC).

Isotopes: Incomplete; no carbon isotopes. Tritium at detection limit (8 TU at this time) and δ^{18}O at –11.50‰ VSMOW.

Trace elements: Poor coverage.

General: Na(Ca)-Cl(HCO$_3$,SO$_4$ brackish groundwater with a small Mg content of 28 mg/L which may suggest a weak marine (Littorina/Baltic?) component.

Comment: Groundwater composition expected at this depth. The second last sample was selected as it was the only one with isotope data. This sample with almost 5% drilling water, together with incomplete isotope data, high tritium detection level and a lack of trace element data, is allocated a Category 3.

C2.1.3 KLX01 (456.00–461.00 m; mid. vertical elevation: –440.73 m)

Cored Borehole					
Category	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					x
Time series (adequate)					x
Time series (inadequate)					
Time series absent					
Suitable section length					x
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					x
Major ions (incomplete)					
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					x
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX05 (19.00–20.00 m). There is no documented sample from the time of drilling borehole KLX01 (i.e. first phase to 703.00 m in 1988 and second phase to 1,077. 99 m in 1990); in the Extended L.2.3 dataset one sample (Experiment Water) is documented from 2003-03-12 and used here. Na-HCO$_3$ type groundwater with low chloride (5.4 mg/L) with enriched δ^{18}O at –9.7‰ V-SMOW and δ^{2}H at –74.4‰ V-SMOW; no tritium or carbon isotope data are available.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –2.52% to –0.15%.

Time Series: 1988-11-08 to 1989-11-23 (15 days). Good series with stable salinity ranging from 1,650–1,700 mg/L Cl, and supported by the remaining major ions. Drilling water high and constant ranging from 13.10–14.00%. Analytical data sporadic for Mn, Li, Sr and DOC with TOC totally lacking, but final sampled groundwater has a good major ion coverage with only TOC absent.

Isotopes: Incomplete isotopes; no carbon isotopes. Tritium detection limit at 8.0 TU and δ^{18}O at –12.2‰ VSMOW.

Trace elements: Lack of data.

General: Na(Ca)-Cl(SO$_4$,HCO$_3$) brackish groundwater. There is less Mg (~ 18 mg/L) than the previous sample indicating no significant Littorina/Baltic component.

Comment: Overall salinity range is low given that the previous section described above at 272.00–277.00 m has around 2,000 mg/L Cl and that below at 680.00–702.11 m has around 4,800 mg/L. Suspected is short circuiting via fractures angled to the surface, such that less saline groundwater may have been drawn into the section from shallower levels and mixed with a groundwater characterised by a more depleted δ^{18}O at –12.2‰ SMOW. The presence of a significant drilling water component may also have entered this level or alternatively introduced during drilling. Furthermore, the groundwater typical for this level may be brackish glacial in origin, and therefore more dilute than expected at this depth. To know the tritium content would have been useful and it is not possible to extrapolate from other KLX01 sections because of the high detection limit. These combined uncertainties have led to the allocation of a Category 5.

C2.1.4 KLX01 (680.00–702.11 m; mid. vertical elevation: –672.95 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)			x		
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)			x		
Time series (inadequate)			x		
Time series absent					
Suitable section length			x		
Sampling during drilling			x		
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)			x?		

Drilling Water: HLX05 (19.00–20.00 m). There is no documented sample from the time of drilling borehole KLX01 (i.e. first phase to 703.00 m in 1988 and second phase to 1,077. 99 m in 1990); in the Extended L.2.3 dataset one sample (Experiment Water) is documented from 2003-03-12 and used here. Na-HCO$_3$ type groundwater with low chloride (5.4 mg/L) with enriched δ^{18}O at –9.7‰ VSMOW and δ^{2}H at –74.4‰ VSMOW; no tritium or carbon isotope data are available.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –3.2% to +0.28% (excluding sample #1514 at –36.25%).

Time Series: Two sampling campaigns from 1988-10-04 to 1988-11-03 (30 days) and from 1989-10-23 to 1989-11-01 (9 days). During the first campaign, salinity increased from 1,670–4,870 mg/L Cl (stabilising during the final 8 days to about 4,850 mg/L Cl) accompanied by a rapid drilling water decrease from 10.4–2.60%. During the second campaign, the salinity increased from 4,140–4,460 mg/L Cl (stabilising during the final 3–4 days), accompanied by a systematic drilling water increase from 1.34 to 1.99%. In both occasions the behaviour of Cl is supported by the remaining major ions. During the first campaign the analytical data is sporadic for Mn, Li, Sr and DOC with TOC totally lacking, but the chosen sampled groundwater has a good major ion coverage with only TOC lacking.

Isotopes: Incomplete isotopes; no carbon isotopes. Tritium below detection (< 8.0 TU); depleted δ^{18}O at –13.3‰ VSMOW for the first campaign indicates a significant cold climate (glacial) component. In contrast, more enriched δ^{18}O at –11.8% VSMOW characterises the second campaign.

Trace elements: Lack of data.

General: Na(Ca)-Cl (SO$_4$) brackish groundwater on both sampling occasions with about 23 mg/L Mg indicating a possible weak marine component. The 1988 sampling occasion appears to represent a brackish glacial groundwater type.

Comment: The overall salinity range is that expected for this depth and during both the 1988 and 1989 sampling the salinity stabilised at around 4,700 and 5,000 mg/L Cl respectively with a constant 2% drilling water. More time series data would have been helpful on both occasions to establish full stability. The high detection level for tritium is problematic and because other KLX01 sections have the same high detection limit, it is not possible to extrapolate a more accurate value. The first sampling campaign was chosen as more representative and this included the selection of the depleted $\delta^{18}O$ value (i.e. glacial component) as being more typical for this depth than the more enriched value (–11.8‰ VSMOW) recorded for the second campaign. Instability (perhaps due to some short circuiting), absence of more quantitative tritium values and a lack of isotopic time series, have allocated this sample to a Category 3.

C2.1.5 KLX01 (830.00–841.00 m; mid. vertical elevation: –817.95 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)				x	
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)				x	
Time series absent					
Suitable section length				x	
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HLX05 (19.00–20.00 m). There is no documented sample from the time of drilling borehole KLX01 (i.e. first phase to 703.00 m in 1988 and second phase to 1,077. 99 m in 1990); in the Extended L.2.3 dataset one sample (Experiment Water) is documented from 2003-03-12 and used here. Na-HCO_3 type groundwater with low chloride (5.4 mg/L) with enriched $\delta^{18}O$ at –9.7‰ VSMOW and δ^2H at –74.4‰ VSMOW; no tritium or carbon isotope data are available.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –1.76% to +0.35% (excluding samples #1758 and #1759 at values of +94.45 and –99.12% respectively.

Time Series: 1990-09-21 to 1990-10-09 (18 days). Time series indicated that apart from the first two Cl values at 9,930 and 9,250 mg/L, the rest of the series showed good stability at 9,200–9,180 mg/L Cl (this is supported by the other major ions). Furthermore, with respect to the drilling water content, apart the first sample which recorded 1.82%, all subsequent samples contained < 1% drilling water. Good major ion coverage apart from an absence of TOC/DOC.

Isotopes: Incomplete isotopes; no carbon isotopes (lack of HCO_3 ~ 6 mg/L). No tritium or $\delta^{18}O$ data recorded, only δ^2H at –96.9‰ VSMOW.

Trace elements: Lack of data.

General: Ca(Na)-Cl(SO_4) brackish non-marine groundwater.

General: Overall salinity range is that expected for brackish non-marine groundwater at this depth. The last sample collected was chosen as more representative based only on available δ^2H data. In general, the groundwater shows good stability, minimal drilling water contamination and almost complete major ion data. However, the absence of key isotope values relegate this sample to a Category 4.

C2.1.6 KLX01 (910.00–921.00 m; mid. vertical elevation: –897.09 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)				x	
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)				x	
Time series absent					
Suitable section length				x	
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Drilling Water: HLX05 (19.00–20.00 m). There is no documented sample from the time of drilling borehole KLX01 (i.e. first phase to 703.00 m in 1988 and second phase to 1,077. 99 m in 1990); in the Extended L.2.3 dataset one sample (Experiment Water) is documented from 2003-03-12 and used here. Na-HCO_3 type groundwater with low chloride (5.4 mg/L) with enriched $\delta^{18}O$ at –9.7‰ VSMOW and δ^2H at –74.4‰ VSMOW; no tritium or carbon isotope data are available.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at –0.94% to +0.81%.

Time Series: 1990-10-12 to 1990-10-30 (18 days). Time series indicated that apart from the first sample at 10,000 mg/L Cl, the remaining series varied from 10,800–11,100 mg/L Cl indicating a small, but nevertheless incremental increase with time (also reflected by the other major ions). More time series data would have been helpful. Apart from the initial sample with 3.84% drilling water, and one later spike of 2.5%, the remaining time series are reasonably steady at 0.73–1.12%. Incomplete major ions: no TOC/DOC.

Isotopes: Incomplete isotopes; no carbon isotopes (lack of HCO_3 ~ 7 mg/L). No tritium or $\delta^{18}O$ data; only δ^2H at –92.9‰ VSMOW.

Trace elements: Lack of data.

General: Ca(Na)–Cl(SO_4) saline groundwater (< 10 mg/L Mg).

Comment: Overall salinity range is that expected for saline groundwater this depth. The last sample collected was chosen based only on available δ^2H data. In general, the groundwater shows some instability (possibly due to short circuiting?), but the major problem is incomplete major ions, an absence of trace elements and key isotope values. Allocated Category 4.

C2.1.7 KLX01 (999.00–1,077.99 m; mid. vertical elevation: –1,019.91 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)				x	
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)				x	
Time series (inadequate)					
Time series absent					
Suitable section length				x	
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HLX05 (19.00–20.00 m). There is no documented sample from the time of drilling borehole KLX01 (i.e. first phase to 703.00 m in 1988 and second phase to 1,077. 99 m in 1990); in the Extended L.2.3 dataset one sample (Experiment Water) is documented from 2003-03-12 and used here. Na-HCO$_3$ type groundwater with low chloride (5.4 mg/L) with enriched δ^{18}O at –9.7‰ VSMOW and δ^{2}H at –74.4‰ VSMOW; no tritium or carbon isotope data are available.

Charge Balance: No measured values given in Sicada but modelled PHREEQC values at +0.19% to +0.92%.

Time Series: 1990-11-05 to 1990-11-19 (14 days). Time series indicated a small variation in salinity with time (12,400–12,600 mg/L Cl) but no systematic change, and this is reflected by the other major ions. In contrast, the drilling water content showed a systematic decrease from 3.18–1.83% during the sampling period. Incomplete major ions, no TOC/DOC.

Isotopes: Incomplete isotopes; no carbon isotopes (lack of HCO$_3$ ~ < 15 mg/L). No tritium or δ^{18}O data recorded, only δ^{2}H at –90.9‰ VSMOW.

Trace elements: Lack of data.

General: Ca-Na-Cl (SO$_4$) saline groundwater (< 10 mg/L Mg).

Comment: Overall salinity range is that expected for saline groundwater at this depth. The last sample collected was chosen based only on available δ^{2}H data Because of incomplete major ions and absence of trace elements and key isotope values, a Category 4 is allocated.

C2.2 Description of Borehole KLX02

Borehole KLX02 was the second and deepest borehole to be drilled at the Laxemar site. Drilling commenced in 1992-08-15 and was completed in 1992-11-29 at a near-vertical depth of 1,700.50 m (vertical depth 1,688.23 m) at an inclination of –84.99° to the horizontal. Percussion drilling was initially carried out to 200.80 m followed by casing to this depth prior to the core drilling phase. The borehole was drilled to complement that of KLX01 and to access deep groundwater sources.

The dominant rock type encountered throughout the borehole is Ävrö granite with numerous zones (some up to 250 m thick) of fine-grained dioritoid mostly between 540–960 m and more minor zones of fine-grained diorite-gabbro (maximum of 200 m) distributed throughout the borehole but mostly between 850–930 m. One major deformation zone is intercepted from about 780–970 m.

Earlier documentation of groundwater quality is given in R-06-12 and R-06-70.

Differential Flow Log: Differential flow log measurements were carried to about 1,400 m depth from March–May, 1999 and hydraulic injection tests to 1,000 m. Borehole KLX02 records significant hydraulic conductivity values mostly in the upper 350 m (maximum to $10^{-5.3}$ ms^{-1} at almost 250 m) and about 1,080–1,160 m which is the greatest depth measured (maximum to about $10^{-6.9}$ ms^{-1}). A further more moderate to low hydraulic conductivity occurs from about 350–1,080 m with values ranging from below detection at 10^{-10} to about $10^{-7.5}$ ms^{-1}. Only at about 550–650 m is there an indication of very low conductivity (i.e. $< 10^{-9}$ ms^{-1}). 'Undisturbed' flow (without pumping) mostly indicates groundwater movement from the borehole to the surrounding bedrock; this is reversed without exception with pumping.

Injection tests to 1,000 m reveal a range of hydraulic conductivity from 10^{-9}–10^{-5} ms^{-1} along the borehole length with the most transmissive section extending from 200 m (extent of the casing) to about 350 m. Groundwater samples from 315.0–321.5 m and 335.0–340.8 m are representative for this borehole section. From 350–1,000 m hydraulic conductivities fluctuate little, averaging around 10^{-9}–$10^{-7.5}$ ms^{-1}; 800–1,000 m depth is also characterised by an increased frequency of open fractures. At these depths groundwaters samples have been collected from 798.0–803.8 m and 1,090–1,096.2 m. Groundwaters were taken also at greater depths: 1,155–1,355 m and 1,420–1,705 m respectively.

Electrical Conductivity log: This was measured both with and without pumping. Without pumping there is no variation in salinity along the borehole (at about 0.04 Sm^{-1}) from 200–1,160 m. From 1,160 m there is a sharp increase to about 2 Sm^{-1} at 1,190 m, and then a more gradual increase to just over 9 Sm^{-1} at 1,400 m, the limit of the measurements. During pumping the pattern changes little for the uppermost 400 m (apart from a small decrease in salinity to about 0.035 Sm^{-1} from 200–270 m), but this is followed by: a) a marked increase in salinity to about 1.4 Sm^{-1} which continues increasing systematically to 2 Sm^{-1} at 1,090 m, b) a sudden increase to 4 Sm^{-1} at 1,100 m, c) an increase to 4.5 Sm^{-1} at 1,160 m, d) a further increase to about 6 Sm^{-1} at 1,170 m, and finally, e) a reasonably constant salinity of 6.5–7.0 Sm^{-1} to 1,400 m. This underlines the necessity for adequate pumping prior to representative groundwater sampling, i.e. to remove the near surface dilute waters which have penetrated downwards during open hole conditions (and also by introduced drilling water) and entered the host bedrock via the intersecting hydraulically conductive fractures and fracture zones.

Comment: Most of the accumulated data from KLX02 indicate the possibility of the following open borehole flow regime /TR-01-11/:

- The upper part of the borehole, about 0–800 m, is more dynamic, i.e. the groundwater turnover time is shorter than in the bottom part of the borehole, section 800–1,700 m.
- Groundwater emerging from the shallow part of the bedrock recharges into the borehole above 200 m borehole length (i.e. between the casing and the borehole). This groundwater continues downward in the open borehole where portions discharge into fractures in the interval 200–800 m, except in a few sections, where flow recharges.
- At about 800 m, the downward moving groundwater encounters a minor, upwardly flowing groundwater flow from the deeper parts of the borehole, i.e. from the interval 800–1,700 m.
- The groundwater of shallow as well as of deep origin discharges into the highly fractured interval at 730–1,120 m.

The conclusion is that shallow groundwater is conducted via borehole KLX02 to greater depths, where mixing with deep groundwater occurs. With time, this process will affect increasingly large groundwater volumes around the borehole, whereby *in situ* conditions will be concealed.

References: SKB TR-01-11, P-04-288, R-06-12, R-06-21.

A major problem is the confidence of the KLX02 groundwater chemistry at depths less than 1,000 m because of the borehole history considerations listed above. It is generally accepted that the water chemistry is perturbed by excessive pumping and an interconnected fracture/borehole system which has circulated groundwater from the near surface to considerable depths.

C2.2.1 KLX02 (315.00–321.00 m; mid. vertical elevation: –298.57 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					x
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					x
Time series absent					
Suitable section length					x
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX10 (0–85 m; mid. vertical elevation: –27.86 m). There is no documented sample from the time of drilling borehole KLX02 from 1992-08-15 to 1992-09-05; in the Extended L.2.3 dataset one sample is documented from 2003-03-12 and used here. Na-HCO_3 type groundwater with low chloride (6.3 mg/L) with $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –78.8‰ VSMOW; tritium at 7.2 TU, $\delta^{13}C$ at –17.45‰ PDB and ^{14}C at 55.73 pmC.

Charge Balance: Measured Sicada values at –3.68% to –0.067%.

Time Series: 1994-01-31 to 1994-02-10 (11 days) showing a somewhat erratic salinity range for the 4 samples (33–73 mg/L Cl) and reflected by Na (74–111 mg/L) and SO_4 (23–46 mg/L); more time series samples would have been helpful. Drilling water consistently < 1%. Major ions complete apart for TOC.

Trace elements: Lacking data.

Isotopes: Incomplete; no carbon isotopes. No tritium values; $\delta^{18}O$ at –10.3‰ VSMOW.

General: Na(Ca)–HCO_3 fresh groundwater.

Comment: Groundwater is only slightly more mineralised than the HLX10 drilling water even at approximately 300 m depth. Suspected short circuiting during sampling from shallower depths, or an artefact of excessive hydraulic pumping carried out following initial drilling. This, combined with an inadequate time series to establish stability and incomplete isotope and trace element data, has resulted in a Category 5 sample.

C2.2.2 KLX02 (335.00–340.80 m; mid. vertical elevation: –318.13 m)

Cored Borehole					
Category	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)					x
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					x
Time series absent					
Suitable section length					x
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX10 (0–85 m; mid. vertical elevation: –27.86 m). There is no documented sample from the time of drilling borehole KLX02 from 1992-08-15 to 1992-09-05; in the Extended L.2.3 dataset one sample is documented from 2003-03-12 and used here. Na-HCO_3 type groundwater with low chloride (6.3 mg/L) with $\delta^{18}O$ at –10.9‰ VSMOW and δ^2H at –78.8‰ VSMOW; tritium at 7.2 TU, $\delta^{13}C$ at –17.45‰ PDB and ^{14}C at 55.73 pmC.

Charge Balance: Measured Sicada values at –2.64% to –0.67%.

Time Series: 1993-11-01 to 1993-11-08 (7 days). Inadequate time series as there is a systematic increase in salinity (126–225 mg/L Cl) during the sampling period reflected by Na, Ca and SO_4; more time may have established stability. Drilling water consistently < 1%. Incomplete major ions: No TOC/DOC.

Isotopes: Incomplete isotopes; no carbon isotopes. No tritium data, $\delta^{18}O$ at –10.60‰ VSMOW.

Trace elements: Lack of data.

General: Na(Ca)-HCO_3 weakly brackish groundwater.

Comment: Groundwater of recharge origin only slightly more mineralised than the HLX10 drilling water even at approximately 320 m depth. Suspected short circuiting from shallow levels during sampling or an artefact of excessive hydraulic pumping carried out following initial drilling. This, combined with inadequate time series to establish stability and incomplete isotope and trace element data, has resulted in a Category 5 allocation.

C2.2.3 KLX02 (452.00–494.00 m; mid. vertical elevation: –452.50 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					x
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					x
Time series absent					
Suitable section length					x
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					x
Major ions (incomplete)					
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					
Monitoring borehole section					x
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX10 (0–85 m; mid. vertical elevation: –27.86 m). There is no documented sample from the time of drilling borehole KLX02 from 1992-08-15 to 1992-09-05; in the Extended L.2.3 dataset one sample is documented from 2003-03-12 and used here. Na-HCO_3 type groundwater with low chloride (6.3 mg/L) with $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –78.8‰ VSMOW; tritium at 7.2 TU, $\delta^{13}C$ at –17.45‰ PDB and ^{14}C at 55.73 pmC.

Charge Balance: Measured Sicada values at +0.89% to +7.70%.

Time Series: Monitoring borehole section sampled on two occasions at 2005-06-14 and 2006-10-31. Within this interval an increase in salinity is indicated (563–645 mg/L Cl) and this is reflected by Na, HCO_3 and SO_4 suggesting an input of shallower groundwater; more time series data are required. Drilling water content decreased from 4.73–1.30%. Major ion coverage complete, although TOC is anomalously high at 150–50 mg/L and Fe(tot) at 15,000–8,500 mg/L when comparing the first and second samples. Contamination suspected.

Isotopes: Complete isotopes; $\delta^{13}C$ at –19.17 to –14.78‰ PDB, ^{14}C at 61.61–61.95 pmC. Tritium at 2.8–3.0 TU and $\delta^{18}O$ at –11.9‰ VSMOW.

Trace elements: Good coverage.

General: Na(Ca)-Cl(SO_4,HCO_3) weak brackish groundwater.

Comment: Overall good coverage of data although missing adequate time series and > 1% drilling water. However, uncertainty still prevails from: a) borehole history considerations, and b) how representative are the data within the monitoring programme due to rapid sampling and lack of time series, and c) short circuiting. Hydraulic tracer tests using uranine as a tracer have been carried out in the same borehole section from 2005-12-08 to 2005-12-15, i.e. prior to the groundwater sampling. The generally low drilling water values recorded would seem to indicate that any marked effects of these tests (i.e. possibly leading an erroneous interpretation of the amount of drilling water) have been removed mostly prior to the groundwater sampling. Allocated Category 5.

C2.2.4 KLX02 (798.00–803.80 m; mid. vertical elevation: –778.18 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					x
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					x
Time series absent					
Suitable section length					x
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX10 (0–85 m; mid. vertical elevation: –27.86 m). There is no documented sample from the time of drilling borehole KLX02 from 1992-08-15 to 1992-09-05; in the Extended L.2.3 dataset one sample is documented from 2003-03-12 and used here. Na-HCO_3 type groundwater with low chloride (6.3 mg/L) with $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –78.8‰ VSMOW; tritium at 7.2 TU, $\delta^{13}C$ at –17.45‰ PDB and ^{14}C at 55.73 pmC.

Charge Balance: Measured Sicada values at –3.14% to –0.05%.

Time Series: 1993-11-11 to 1993-11-23 (12 days). Inadequate time series data showing salinity fluctuations (from 87–717 mg/L Cl), reflected also for the other major ions. Drilling water content is consistently < 1% during the sampling period. Major ions incomplete; no TOC for the final sample collected.

Isotopes: Incomplete isotopes; no carbon isotopes. No tritium, $\delta^{18}O$ at –10.9‰ VSMOW.

Trace elements: Lack of data.

General: Na(Ca)–Cl(HCO_3,SO_4) weakly brackish groundwater.

Comment: Uncertainty still prevails from borehole history considerations; still unusually dilute for such depths which may indicate short circuiting with shallower bedrock environments. This dilution, plus instability (more time series data required) and a lack of carbon and tritium isotopic data, all point to the allocation of a Category 5.

C2.2.5 KLX02 (1,090.00–1,096.20 m; mid. vertical elevation: –1,068.24 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)			x		
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)			x		
Time series (inadequate)					
Time series absent					
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HLX10 (0–85 m; mid. vertical elevation: –27.86 m). There is no documented sample from the time of drilling borehole KLX02 from 1992-08-15 to 1992-09-05; in the Extended L.2.3 dataset one sample is documented from 2003-03-12 and used here. Na-HCO_3 type groundwater with low chloride (6.3 mg/L) with $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –78.8‰ VSMOW; tritium at 7.2 TU, $\delta^{13}C$ at –17.45‰ PDB and ^{14}C at 55.73 pmC.

Charge Balance: Measured Sicada values at –2.03% to +2.36%.

Time Series: 1993-12-02 to 1993-12-16 (14 days) showing a systematic increase during the sampling period from 12,300–15,800 mg/L Cl, levelling out during the last 3 days. Increases are recorded also by Na and SO_4 and a decrease in HCO_3. Drilling water content is consistently < 1% during this sampling period. Major ion coverage is sporadic for the time series, and incomplete for the last sample collected, i.e. for Fe(tot), Fe^{2+} and TOC, although values can be extrapolated from the rest of the time series.

Isotopes: Incomplete isotopes; no carbon isotopes (lack of HCO_3 ~ < 10 mg/L). No tritium data and a single $\delta^{18}O$ value at –11.7‰ VSMOW for the last sample collected.

Trace elements: Lack of data.

General: Ca(Na)-Cl(SO_4) saline groundwater.

Comment: Chemical instability is evident during the initial stages of sampling, but the final sample collected is considered quite representative. Despite the absence of much of the isotope data, the < 1% drilling water and the fact that the major ion groundwater chemistry is what is expected at this depth, a Category 3 is allocated.

C2.2.6 KLX02 (1,090.00–1,097.00 m; mid. vertical elevation: –1,068.64 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					–
Drilling water (≤ 5%)					–
Drilling water (≤ 10%)					–
Drilling water (> 10%)					–
Time series (adequate)					
Time series (inadequate)					x
Time series absent					
Suitable section length					x
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HLX10 (0–85 m; mid. vertical elevation: –27.86 m). There is no documented sample from the time of drilling borehole KLX02 from 1992-08-15 to 1992-09-05; in the Extended L.2.3 dataset one sample is documented from 2003-03-12 and used here. Na-HCO_3 type groundwater with low chloride (6.3 mg/L) with $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –78.8‰ VSMOW; tritium at 7.2 TU, $\delta^{13}C$ at –17.45‰ PDB and ^{14}C at 55.73 pmC.

Charge Balance: Measured Sicada values at +0.11% to +3.04%.

Time Series: Almost the same borehole section described above sampled six years later from 1999-09-27 to 1999-10-28 (31 days). Compared with the previous data, this shows a much less saline groundwater with a systematic increase during the sampling period from 1,010–4,730 mg/L Cl, and greater amounts of HCO_3 and Mg (up to 25 mg/L) which suggests contact with a much more dilute shallow groundwater with a weak marine signature. Drilling water content was not measured. Inadequate time series data. Major ions complete apart from TOC.

Isotopes: Complete isotopes; $\delta^{13}C$ at –21.50‰ PDB, ^{14}C at 68.90 pmC. Tritium at 8.4–11.5 TU and $\delta^{18}O$ values at –10.90 to –10.4‰ VSMOW.

Trace elements: Good coverage.

General: Ca(Na)-Cl(SO_4) brackish groundwater.

Comment: Completely different groundwater than six years previously from the same borehole section. During this time open hole conditions have led to younger waters descending the borehole and mixing with different groundwater types (some with a marine signature) to produce brackish groundwaters which are not representative for this level. Allocated Category 5.

C2.2.7 KLX02 (1,145.00–1,164.00 m; mid. vertical elevation: –1,129.14 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)				x	
Drilling water (≤ 5%)					
Drilling water (≤ 10%)				?	
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)				x	
Time series absent					
Suitable section length				x	
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)				x	
Major ions (incomplete)					
Environmental isotopes (complete)				x	
Environmental isotopes (incomplete)					
Monitoring borehole section				x	
Hydraulic effects (short circuiting)					

Drilling Water: HLX10 (0–85 m; mid. vertical elevation: –27.86 m). There is no documented sample from the time of drilling borehole KLX02 from 1992-08-15 to 1992-09-05; in the Extended L.2.3 dataset one sample is documented from 2003-03-12 and used here. Na-HCO_3 type groundwater with low chloride (6.3 mg/L) with $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –78.8‰ VSMOW; tritium at 7.2 TU, $\delta^{13}C$ at –17.45‰ PDB and ^{14}C at 55.73 pmC.

Charge Balance: Measured Sicada values at –1.18% to +0.66%.

Time Series: Monitoring borehole section close to the same borehole section sampled at 1,090.00–1,096.20 m 13–14 years previously. Sampled on three occasions in 2006-06-21, 2006-10-31 and 2007-07-10 and shows acceptable stability at about 15,000 mg/L Cl; this is also reflected by the other major ions. Drilling water is < 1% for two sampling occasions but up to 10.20% in the October 31st 2006 sampling occasion. Complete major ions.

Isotopes: Complete isotopes; no carbon isotopes (due to a lack of HCO_3 ~ 21 mg/L). Tritium at 1.2–3.8 TU and slightly depleted $\delta^{18}O$ values at –12.0‰ VSMOW.

Trace elements: Good coverage.

General: Ca(Na)-Cl(SO_4) saline groundwater.

Comment: This groundwater is almost identical to that of level 1,090.00–1,096.20 m. Good chemical stability, adequate time series and good coverage of major ions and trace elements. Uncertainty associated with the tritium contents at this depth. With a < 1% drilling water component this is an unlikely source; other potential contamination sources cannot be ruled out, e.g. sampling pump system (cf. section 3.1.1).

This section has also been the location for hydraulic tracer tests using uranine (and therefore the possibility of erroneously calculated drilling water contents) from 2005-12-09 to 2005-12-25 and 2006-11-23 to 2006-11-28, and using rhodamine and HLX10 groundwater in 2004-07-27. The first and third sampling occasions appear to be virtually unaffected recording < 1% drilling water, but the third occasion in 2007-07-10 records 10.2% drilling water which can be correlated with the uranine tracer tests carried out in 2006-11-23.

More time series data would have been required and an additional problem is how representative are the data within the monitoring programme. Allocated Category 4. (Note: this sample supports the Category 3 category given to borehole section 1,090.00–1,096.20 m).

C2.2.8 KLX02 (1,155.00–1,165.00 m; mid. vertical elevation: –1,134.60 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					–
Drilling water (≤ 5%)					–
Drilling water (≤ 10%)					–
Drilling water (> 10%)					–
Time series (adequate)					
Time series (inadequate)					x
Time series absent					
Suitable section length					x
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					x
Major ions (incomplete)					
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HLX10 (0–85 m; mid. vertical elevation: –27.86 m). There is no documented sample from the time of drilling borehole KLX02 from 1992-08-15 to 1992-09-05; in the Extended L.2.3 dataset one sample is documented from 2003-03-12 and used here. Na-HCO_3 type groundwater with low chloride (6.3 mg/L) with $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –78.8‰ VSMOW; tritium at 7.2 TU, $\delta^{13}C$ at –17.45‰ PDB and ^{14}C at 55.73 pmC.

Charge Balance: Measured Sicada values at –2.06% to +1.05%.

Time Series: Present section is close to the previously described three borehole sections. It was sampled from 1999-09-01 to 1999-09-15 (14 days) showing a small but systematic increase in salinity from 14,220–15,130 mg/L Cl; this was accompanied by an increase in SO_4 (766–860 mg/L) and Na (3,700–3,730 m g/L) and a small decrease in Ca (5,300–5,250 mg/L. No measurements of drilling water are documented. Incomplete major ions; no TOC.

Isotopes: Complete isotopes; no carbon isotopes (lack of HCO_3 contents < 20 mg/L). Tritium at 1.8–2.6 TU and $\delta^{18}O$ values at –11.4‰ VSMOW.

Trace elements: Reasonable coverage of REEs.

General: Ca(Na)-Cl(SO_4) saline groundwater.

Comment: Groundwater is almost identical to that of the previous three levels but there is a lack of chemical stability that additional time series may have solved. Uncertainty associated with the tritium contents at this depth but not possible to check because no drilling water data; anthropogenic contamination from pumping equipment can be ruled out because of pre-2000 sampling. Allocated Category 5.

C2.2.9 KLX02 (1,345.00–1,355.00 m; mid. vertical elevation: –1,322.81 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)			–		
Drilling water (≤ 5%)			–		
Drilling water (≤ 10%)			–		
Drilling water (> 10%)			–		
Time series (adequate)					
Time series (inadequate)			x		
Time series absent					
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)			x		
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HLX10 (0–85 m; mid. vertical elevation: –27.86 m). There is no documented sample from the time of drilling borehole KLX02 from 1992-08-15 to 1992-09-05; in the Extended L.2.3 dataset one sample is documented from 2003-03-12 and used here. Na-HCO_3 type groundwater with low chloride (6.3 mg/L) with $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –78.8‰ VSMOW; tritium at 7.2 TU, $\delta^{13}C$ at –17.45‰ PDB and ^{14}C at 55.73 pmC.

Charge Balance: Measured Sicada values at –4.03% to –0.97%.

Time Series: 1999-07-19 to 1999-08-10 (22 days) showing a small systematic increase in salinity from 31,060–31,590 mg/L Cl; Na and Ca show a small decrease during the final sampling period. More time series would have been helpful. No measurements of drilling water have been documented. Incomplete major ions; no TOC.

Isotopes: Complete isotopes; no carbon isotopes (lack of HCO_3 ~ 9–16 mg/L). Tritium under detection (< 0.8 TU), and enriched $\delta^{18}O$ ranging from –9.7 to –9.3‰ VSMOW.

Trace elements: Reasonable coverage of REEs.

General: Ca(Na)-Cl(SO_4) highly saline groundwater.

Comment: Groundwater composition is expected at this depth; increased water/rock interaction processes is supported by the enriched $\delta^{18}O$ values (i.e. compare to the previous levels around 1,000 m depth where a small glacial component may be present). However, the absence of drilling water values introduce some uncertainty; this, together with inadequate time series measurements, lead to the allocation of a Category 3.

C2.2.10 KLX02 (1,385.00–1,392.00 m; mid. vertical elevation: –1,360.93 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)				–	
Drilling water (≤ 5%)				–	
Drilling water (≤ 10%)				–	
Drilling water (> 10%)				–	
Time series (adequate)					
Time series (inadequate)				x	
Time series absent					
Suitable section length				x	
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)				x	
Major ions (incomplete)					
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HLX10 (0–85 m; mid. vertical elevation: –27.86 m). There is no documented sample from the time of drilling borehole KLX02 from 1992-08-15 to 1992-09-05; in the Extended L.2.3 dataset one sample is documented from 2003-03-12 and used here. Na-HCO_3 type groundwater with low chloride (6.3 mg/L) with $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –78.8‰ VSMOW. Tritium at 7.2 TU, $\delta^{13}C$ at –17.45‰ PDB and ^{14}C at 55.73 pmC.

Charge Balance: Measured Sicada value at –0.18%.

Time Series: Section is sampled once in 1999-12-06; inadequate time series. Salinity is 36,970 mg/L Cl and no drilling water was measured. HCO_3 is higher than expected at 42 mg/L when compared to similar depths. Incomplete major ions; no TOC.

Isotopes: Incomplete isotopes; no $\delta^{13}C$ but ^{14}C at 76.40 pmC. Tritium at 0.8 TU and enriched $\delta^{18}O$ at –9.3‰ VSMOW.

Trace elements: Reasonable coverage of REEs.

General: Ca(Na)-Cl(SO_4) highly saline groundwater.

Comment: Groundwater salinity content is expected at this depth; increased water/rock interaction processes is supported by the enriched $\delta^{18}O$ values. However, no drilling water values introduce some uncertainty; this, together with inadequate time series measurements and an unexpected high ^{14}C, lead to the allocation of a Category 4.

C2.2.11 KLX02 (1,420.00–1,700.50 m; mid. vertical elevation: –1,530.98 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)			x		
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)			x		
Time series (inadequate)					
Time series absent					
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HLX10 (0–85 m; mid. vertical elevation: –27.86 m). There is no documented sample from the time of drilling borehole KLX02 from 1992-08-15 to 1992-09-05; in the Extended L.2.3 dataset one sample is documented from 2003-03-12 and used here. Na-HCO_3 type groundwater with low chloride (6.3 mg/L) with $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –78.8‰ VSMOW; tritium at 7.2 TU, $\delta^{13}C$ at –17.45‰ PDB and ^{14}C at 55.73 pmC.

Charge Balance: Measured Sicada values at –0.85% to +2.86%.

Time Series: 1993-12-22 to 1994-01-18 (27 days) showing stability ranging from 45,400–46,000 mg/L Cl after the first 6–7 day period; following this values of 29,100–42,200 mg/L Cl are recorded. Variations in Cl are supported by the remaining major ions. Adequate time series. Drilling water when measured was < 1% and shows a systematic decrease with sampling time from 0.46–0.14%. Incomplete major ions: no TOC.

Isotopes: Incomplete isotopes; no carbon isotopes (lack of HCO_3 ~ 8–12 mg/L). Tritium not measured; enriched $\delta^{18}O$ value at –8.9‰ VSMOW.

Trace elements: Lack of data.

General: Ca(Na)-Cl(SO_4) highly saline groundwater.

Comment: Salinity content is expected at this depth; increased water/rock interaction processes is supported by the enriched $\delta^{18}O$ values. However, the absence of tritium values and general lack of time series isotopic data, together with a long sampled section at around 280 m (subject to groundwater mixing from more than one source), indicate a Category 3.

KLX02: Tube samples sampled every 50 m from 9–1,681 m (1993-08-03) and 0–1,450 m (1997-09-25) are considered unrepresentative and allocated Category 5.

C2.3 Description of Borehole KLX03

Borehole KLX03 (a designated chemistry borehole) is 1,000.42 m long (vertical depth 970.69 m), cased to 100.35 m, and inclined at –74.92° from the horizontal. The borehole was drilled from 2004-05-28 to 2004-03-06 to obtain detailed geological, hydrogeological and hydrochemical information from the Ävrö granite/quartz monzodiorite contact area close to deformation zone ZSMNE942A. The dominant rock type intercepted by the borehole is Ävrö granite (containing small zones mostly of diorite/gabbro) from the surface to about 620 m, and then quartz monzodiorite (with zones mostly of fine-grained dioritoid, Ävrö granite and fine-grained granite) to the end of the borehole.

Differential Flow Log: Measurements in borehole KLX03, carried out from 2004-11-04 to 2004-11-18, reveal a general distribution of hydraulic transmissivity from 10^9 (lower detection limit) to 10^5 m^2s^{-1}; areas of greatest transmissivity are located between 100–300 m and 700–800 m, with slightly less (10^9–$10^{6.5}$ m^2s^{-1}) at around 400–450 m, 650 m and 975 m. Under 'natural conditions' (i.e. no pumping) the groundwater flow is from the borehole to the surrounding bedrock with a maximum measured flow rate of 10^4 mL h^{-1} at around 750 m. With pumping the groundwater flow is from the bedrock towards the borehole, with the variation in measured groundwater flow rates (10^2–$10^{5.5}$ mL h^{-1}) closely reflecting the variation of transmissivity in the surrounding bedrock. Between 950–1,000 m there is only a measureable flow rate (10^4 mL h^{-1}) during pumping.

Electrical Conductivity log: The hydraulic complexity of the open borehole conditions is further supported by the electrical conductivity log. During natural flow conditions (i.e. without pumping) an almost uniform dilute chemistry to around 750 m is shown (0.15–0.2 Sm^{-1}), followed by a sharp increase in salinity to 3 Sm^{-1} which continues to the borehole bottom. This indicates three possibilities: a) input of dilute groundwater from the upper part of the borehole of greatest transmissivity (100–450 m) has penetrated to 750 m, b) the depth of the dilute water accurately reflects the extent of dilute formation groundwater in the surrounding bedrock, and c) the input of highly saline water from near the borehole bottom dominates to 750 m.

During pumping, however, there is a marked increase in salinity to 1.2–1.5 Sm^{-1} with the removal of dilute water from around 200 m to approximately 750 m. In contrast, there is no difference from 850 m to the borehole bottom. This indicates that: a) the chemistry of the highly saline groundwater at depth appears to be quite stable and thus probably representative, and b) the dilute borehole waters do not reflect the chemistry of the formation groundwaters to 750 m depth. There is support, therefore, for the intrusion of dilute groundwater into the borehole from the upper, more transmissive, bedrock. Under open hole conditions this dilute water has moved into the surrounding bedrock where higher transmissivities allow, and has been subsequently removed during pumping to be replaced by more saline formation groundwaters. The question is whether enough water has been removed to reveal the true formation groundwater salinity.

Hydrochemical logging: Measurement of the borehole was carried out on 2004-09-21, about 4.5 months prior to the differential flow measurements. Compared to the flow measurements, the hydrochemical logging shows a higher range of electrical conductivity values (0.22–0.38 Sm^{-1}) to a shallower depth from 100–400 m, followed by a higher range (~ 0.6–0.8 Sm^{-1}) from 400–800 m, finally achieving a maximum of 2.34 Sm^{-1} at 990 m depth. This indicates, as inferred above from the flow measurements, that during open hole conditions between the hydrochemical logging and the differential flow measurements, dilute waters have penetrated to a greater depth along the borehole (from about 400–750 m) and the deepest parts of the borehole have become more saline.

The amount of drilling water in the borehole at this stage ranged from 8.0–20.0% from 0–400 m, followed by an increase to a maximum of 60.5% at 740 m, and finally a decrease to 10.2% at 990 m. The total variation in chloride along the borehole is 575–8,720 mg/L, i.e. brackish type groundwater mix.

Comment: The measured high transmissivities relate to the several deformation zones intercepted by KLX03 which, in turn, control the variation in salinity measured under natural and controlled conditions. Due to the high transmissive deformation zones, much of this drilling water mixed with different groundwater sources (mostly from shallow to intermediate depths) have entered the higher transmissive rock mass from the borehole during drilling and subsequently under open hole conditions. These waters will first have to be removed with great care before 'representative' groundwater can be accessed. Short circuiting therefore may be a major problem.

References: SKB P-04-299, P-05-67, P-05-89, P-06-08, R-06-12, R-06-21.

C2.3.1 KLX03 (103.00–218.02 m; mid. vertical elevation: –136.57 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					x
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					x
Time series absent					
Suitable section length					
Sampling during drilling					x
Sampling using PLU hydraulic testing equipment					x
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX14 (11.90–115.90 m; mid. vertical elevation: –29.25 m; major flow input at ~ 85.18 m borehole length). There is no documented drilling water sample taken during the drilling of borehole KLX03 from 2004-05-28 to 2004-09-07; in the Extended L.2.3 dataset one sample is documented from 2004-05-07 and used here. Typical Na-HCO$_3$ fresh recharge groundwater (69.7 mg/L Cl) with a δ^{18}O signature of –11.20‰ VSMOW. Tritium data suggest some younger, near-surface mixing (3.8 TU). (Note: later sampled groundwater from the same borehole is more mineralised).

Charge Balance: Measured Sicada value at –5.80%.

Time Series: Only one sample taken using PLU hydraulic testing equipment during drilling in 2004-06-04. Groundwater is brackish (507 mg/L Cl) with a drilling water content of 1.02%. Major ions incomplete; no F, Fe(tot), Fe(II), S^{2-} or TOC.

Isotopes: Complete; δ^{13}C at –17.18‰ PDB, ^{14}C at 42.7 pmC. Tritium below detection (< 0.8TU), and δ^{18}O at –12.7‰ VSMOW suggests a weak glacial signature.

Trace elements: Lack of data.

General: Na-Cl(HCO$_3$) brackish groundwater with a weak glacial signature.

Comment: Problem with a lack of time series, long borehole section (115 m) possibly facilitating mixing/short circuiting from different groundwater sources, incomplete major ion data and an absence of trace elements. Allocated Category 5.

C2.3.2 KLX03 (193.50–198.37 m; mid. vertical elevation: –170.82 m)

Cored Borehole Category	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)	x				
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)	x				
Time series (inadequate)					
Time series absent					
Suitable section length	x				
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)	x				
Major ions (complete)	x				
Major ions (incomplete)					
Environmental isotopes (complete)	x				
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HLX14 (11.90–115.90 m; mid. vertical elevation: –29.25 m; major flow input at ~ 85.18 m borehole length). There is no documented drilling water sample taken during the drilling of borehole KLX03 from 2004-05-28 to 2004-09-07; in the Extended L.2.3 dataset one sample is documented from 2004-05-07 and used here. Typical Na-HCO$_3$ fresh recharge groundwater (69.7 mg/L Cl) with a δ^{18}O signature of –11.20‰ VSMOW. Tritium data suggest some younger, near-surface mixing (3.8 TU). (Note: later sampled groundwater from the same borehole is more mineralised).

Charge Balance: Measured Sicada values at –1.67% to +0.27%.

Time Series: 2004-11-29 to 2004-12-15 (16 days). Adequate time series; slight decrease in salinity with time (279–259 mg/L Cl) but steady during the final 8–9 days. Drilling water consistently < 1%. Major ions incomplete; no TOC.

Isotopes: Complete isotopes; δ^{13}C at –16.96 to –16.68‰ PDB, ^{14}C at 45.18 to 45.68 pmC. Tritium under detection (< 0.8TU) and δ^{18}O at –11.70 to –11.50‰ VSMOW.

Trace elements: Good coverage.

General: Na-Cl(HCO$_3$) brackish groundwater of shallow origin.

Comment: Adequate time series and stable chemistry, < 1% drilling water, almost complete major ions and trace elements; considered representative for this level. Allocated Category 1.

C2.3.3 KLX03 (408.00–415.30 m; mid. vertical elevation: –379.85 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)			x		
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)			x		
Time series (inadequate)					
Time series absent					
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)			x		
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HLX14 (11.90–115.90 m; mid. vertical elevation: –29.25 m; major flow input at ~ 85.18 m borehole length). There is no documented drilling water sample taken during the drilling of borehole KLX03 from 2004-05-28 to 2004-09-07; in the Extended L.2.3 dataset one sample is documented from 2004-05-07 and used here. Typical Na-HCO_3 fresh recharge groundwater (69.7 mg/L Cl) with a $\delta^{18}O$ signature of –11.20‰ VSMOW. Tritium data suggest some younger, near-surface mixing (3.8 TU). (Note: later sampled groundwater from the same borehole is more mineralised).

Charge Balance: Measured Sicada values at +0.97% to +2.12%.

Time Series: 2005-02-21 to 2005-03-22 (29 days). Adequate time series; slight saline instability during the sampling period but steady (1,410–1,390 mg/L Cl) during the final 8–9 days. Drilling water is consistently < 4%. Major ions complete.

Isotopes: Complete isotopes; $\delta^{13}C$ at –27.10‰ PDB, ^{14}C at 65.20 pmC. Tritium not measured on the selected sample but all others show below detection (< 0.8TU); $\delta^{18}O$ constant at –13.30‰ VSMOW signifying a glacial component.

Trace elements: Good coverage.

General: Na(Ca)-Cl(HCO_3,SO_4) brackish glacial groundwater.

Comment: Adequate time series and stable chemistry, < 5% drilling water, complete major ions and trace elements. However, the absence of a tritium value for the chosen sample has relegated a potential Category 2 to a Category 3.

C2.3.4 KLX03 (497.02–599.89 m; mid. vertical elevation: –512.79 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					x
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					
Sampling during drilling					x
Sampling using PLU hydraulic testing equipment					x
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX14 (11.90–115.90 m; mid. vertical elevation: –29.25 m; major flow input at ~ 85.18 m borehole length). There is no documented drilling water sample taken during the drilling of borehole KLX03 from 2004-05-28 to 2004-09-07; in the Extended L.2.3 dataset one sample is documented from 2004-05-07 and used here. Typical Na-HCO_3 fresh recharge groundwater (69.7 mg/L Cl) with a $\delta^{18}O$ signature of –11.20‰ VSMOW. Tritium data suggest some younger, near-surface mixing (3.8 TU). (Note: later sampled groundwater from the same borehole is more mineralised).

Charge Balance: Measured Sicada value at –4.39%.

Time Series: Only one sample taken using PLU hydraulic testing equipment during drilling in 2004-08-14. Groundwater is brackish (381 mg/L Cl) with a drilling water content of 5.15%. Major ions incomplete; no F, Fe(tot), Fe(II), S^{2-} or TOC.

Isotopes: Complete isotopes; $\delta^{13}C$ at –16.32‰ PDB, ^{14}C at 47.52 pmC. Tritium under detection (< 0.8 TU) and $\delta^{18}O$ at –11.70‰ VSMOW.

Trace elements: Lack of data.

General: Na-Cl(HCO_3) groundwater.

Comment: Problem with a lack of time series, presence of ~ 5% drilling water, long borehole section (100 m) possibly facilitating mixing/short circuiting different groundwater sources, incomplete major ion data and an absence of trace elements. Allocated Category 5.

C2.3.5 KLX03 (692.86–761.11 m; mid. vertical elevation: –686.22 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					x
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					x
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX14 (11.90–115.90 m; mid. vertical elevation: –29.25 m; major flow input at ~ 85.18 m borehole length). There is no documented drilling water sample taken during the drilling of borehole KLX03 from 2004-05-28 to 2004-09-07; in the Extended L.2.3 dataset one sample is documented from 2004-05-07 and used here. Typical Na-HCO_3 fresh recharge groundwater (69.7 mg/L Cl) with a $\delta^{18}O$ signature of –11.20‰ VSMOW. Tritium data suggest some younger, near-surface mixing (3.8 TU). (Note: Later sampled groundwater from the same borehole is more mineralised).

Charge Balance: Measured Sicada value at –2.97%.

Time Series: Only one sample taken using PLU hydraulic testing equipment during drilling in 2004-08-23. Groundwater is brackish (3,550 mg/L Cl) with a drilling water content of 30.30%. Major ions incomplete, no F, Fe(tot), Fe(II), S^{2-} or TOC.

Isotopes: Incomplete isotopes; no carbon isotopes. Tritium at 1.5 TU and $\delta^{18}O$ at –13.10‰ VSMOW indicating a weak glacial signature.

Trace elements: Lack of data.

General: Na(Ca)-Cl(SO_4) brackish glacial groundwater.

General: Problem with a lack of time series, presence of high drilling water, long borehole section (about 70 m) possibly facilitating mixing/short circuiting different groundwater sources, incomplete major ion data and an absence of trace elements. Category 5 allocated.

C2.3.6 KLX03 (729.00–751.00 m; mid. vertical elevation: –698.88 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)				x	
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					x
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)				x	
Time series absent					x
Suitable section length				x	x
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					x
Major ions (incomplete)					
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					
Monitoring borehole section					x
Hydraulic effects (short circuiting)					?

Drilling Water: HLX14 (11.90–115.90 m; mid. vertical elevation: –29.25 m; major flow input at ~ 85.18 m borehole length). There is no documented drilling water sample taken during the drilling of drilling borehole KLX03 from 2004-05-28 to 2004-09-07; in the Extended L.2.3 dataset one sample is documented from 2004-05-07 and used here. Typical Na-HCO_3 fresh recharge groundwater (69.7 mg/L Cl) with a $\delta^{18}O$ signature of –11.20‰ VSMOW. Tritium data suggest some younger, near-surface mixing (3.8 TU). (Note: later sampled groundwater from the same borehole is more mineralised).

Charge Balance: Measured Sicada value at –0.89%.

Time Series: Only one sample taken from monitoring borehole section in 2006-11-28. Inadequate time series. Groundwater is brackish (1,660 mg/L Cl) with a drilling water content of 8.33%. Major ions complete.

Isotopes: Complete isotopes; $\delta^{13}C$ at –18.08‰ PDB, ^{14}C at 49.98 pmC. Tritium under detection (< 0.8 TU) and $\delta^{18}O$ at –12.60‰ VSMOW.

Trace elements: Good coverage.

General: Na(Ca)-Cl(HCO_3,SO_4) brackish groundwater with a weak glacial component. Problem with a lack of time series, and a salinity that should be greater than that from shallower levels (e.g. compare 1,660 mg/L Cl with 3,550 mg/L Cl from section 692.86–761.11 m). Short circuiting may have contributed. Furthermore, near vicinity borehole levels (740.7–744.4 m and 769.7–772.7 m) have been used for hydraulic tracer tests in 2005 using uranine as a tracer. The high drilling water content measured (8.33%) could possibly be an artefact of the uranine still in the system during groundwater sampling. Allocated Category 5.

C2.3.7 KLX03 (735.50–748.04 m; mid. vertical elevation: –700.60 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					x
Time series (adequate)					x
Time series (inadequate)					
Time series absent					
Suitable section length					x
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					x
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					x
Major ions (incomplete)					
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX14 (11.90–115.90 m; mid. vertical elevation: –29.25 m; major flow input at ~ 85.18 m borehole length). There is no documented drilling water sample taken during the drilling of borehole KLX03 from 2004-05-28 to 2004-09-07; in the Extended L.2.3 dataset one sample is documented from 2004-05-07 and used here. Typical Na-HCO_3 fresh recharge groundwater (69.7 mg/L Cl) with a $\delta^{18}O$ signature of –11.20‰ VSMOW. Tritium data suggest some younger, near-surface mixing (3.8 TU). (Note: later sampled groundwater from the same borehole is more mineralised).

Charge Balance: Measured Sicada values at –2.49% to +1.17%.

Time Series: 2005-04-01 to 2005-04-25 (24 days). Adequate time series; increase in salinity with time (579–1,090 mg/L Cl) reflected also by increases in Na, Ca, SO_4 and drilling water content (6.83–10.80%), a decrease in HCO_3 and an increase in depleted $\delta^{18}O$. Major ions complete.

Isotopes: Complete isotopes; $\delta^{13}C$ at –15.34 to –15.89‰ PDB, ^{14}C at 47.36 to 48.23 pmC. Tritium from under detection (< 0.8 TU) to 1.3 TU, and $\delta^{18}O$ at –13.60‰ VSMOW indicates a significant glacial component.

Trace elements: Reasonably good coverage.

General: Change to a more evolved Ca(Na)-Cl(SO_4,HCO_3) brackish glacial groundwater.

Comment: Adequate time series but chemistry is unstable due to the systematic change in composition with time by a more saline brackish glacial groundwater component mixed with an increasing amount of drilling water, possibly due to short circuiting processes. It is doubtful that more time series measurements would have achieved stability. Furthermore, as mentioned in the above described sample, near vicinity borehole levels (740.7–744.4 m and 769.7–772.7 m) have been used for hydraulic tracer tests in 2005 using uranine as a tracer. The high drilling water content measured (8.33%) could possibly be an artefact of the uranine still in the system during groundwater sampling. Allocated Category 5.

C2.3.8 KLX03 (964.50–975.15 m; mid. vertical elevation: –922.45 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)	x				
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)	x				
Time series (inadequate)					
Time series absent					
Suitable section length	x				
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)	x				
Major ions (complete)	x				
Major ions (incomplete)					
Environmental isotopes (complete)	x				
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HLX14 (11.90–115.90 m; mid. vertical elevation: –29.25 m; major flow input at ~ 85.18 m borehole length). There is no documented drilling water sample taken during the drilling of borehole KLX03 from 2004-05-28 to 2004-09-07; in the Extended L.2.3 dataset one sample is documented from 2004-05-07 and used here. Typical Na-HCO_3 fresh recharge groundwater (69.7 mg/L Cl) with a $\delta^{18}O$ signature of –11.20‰ VSMOW. Tritium data suggest some younger, near-surface mixing (3.8 TU). (Note: later sampled groundwater from the same borehole is more mineralised).

Charge Balance: Measured values at +0.86% +1.32%.

Time Series: 2005-01-24 to 2004-02-14 (21 days). Adequate time series and reasonably good stability although a small increase in salinity with time if the first sample is ignored (10,400–10,500 mg/L Cl); drilling water content is consistently < 1% during the sampling period. Complete major ions.

Isotopes: Complete isotopes; no carbon isotopes (lack of HCO_3 < 20 mg/L). Tritium under detection (< 0.8TU) and $\delta^{18}O$ at –12.20‰ VSMOW.

Trace elements: Reasonably good coverage.

General: Ca(Na)-Cl(SO_4) saline groundwater with a possible weak glacial signature.

Comment: Adequate time series and overall chemical stability, < 1% drilling water and complete major ion and most trace elements. Allocated Category 1.

KLX03: Tube samples sampled every 50 m from 00.00–915.00 m (2004-09-21) are considered unrepresentative and allocated Category 5.

C2.4 Description of Borehole KLX04

Borehole KLX04 is 993.49 m long (vertical depth of 988.09 m), cased to 100.35 m, and inclined at –84.68° from the horizontal. Drilling of the borehole, to obtain detailed geological and hydrogeological and information, lasted from 2004-03-13 to 2004-06-28. Borehole KLX04 penetrates a relatively homogeneous rock mass dominated by Ävrö granite. Several sections of quartz monzodiorite occur between approximately 400–550 m and 680–710 m. Granite (medium grained) dominates below 900 m down to the bottom of the borehole. Thin zones of gabbro and fine-grained dioritoid occur along the borehole. Large lengths of the drillcore show fracture frequencies around 2–5 open fractures m^{-1} at 200 to 450 m and 500 to 700 m. Lower fracture frequency is found in the upper 100–200 m and in the section between 700–860 m. The highest frequency of open fractures (5–10 m^{-1}) is found at the bottom of the borehole between 870–980 m.

Two major deformation zones are intersected by KLX04: a) ZMNW929A at 873–973 m (and in KLX02 at 774–935 m), and b) ZSMEW007A at 346–355 m (and in KLX02 at 265–275 m and in KLX01 at 1,000–1,020 m).

Differential Flow Log: Measurements carried out in borehole KLX04 between 2004-07-26 to 2004-08-06 reveal high transmissivities from 100–650 m borehole length ($10^{5.5}$–$10^{4.6}$ m^{2}s^{-1}) with the maximum at 200–300 m. From 650–880 m transmissivities are below detection (10^9 m^{2}s^{-1}) and then increase to a maximum of about 10^7 m^{2}s^{-1} at 880–980 m. Under 'natural conditions' (i.e. no pumping) the groundwater flow is from the borehole to the surrounding bedrock with a maximum measured flow rate of approximately 10^5 mL min^{-1} at 300 m; at 880–980 m the flow rate is 10^3 mL min^{-1}. With pumping the groundwater flow is reversed towards the borehole, the variation in groundwater flow rates (10^2–$10^{5.5}$ mL min^{-1}) closely reflecting the variation of transmissivity in the surrounding bedrock. Slightly higher hydraulic conductivity values are reported from the injection tests when compared to the differential flow measurements.

These observations suggest that during open borehole conditions, the upper approximately 650 m of the borehole in particular and to a lesser extent between 880–980 m, groundwater will preferentially move into the surrounding bedrock. With pumping, for example during sampling, this water will first have to be removed before 'representative' groundwater can be accessed.

Electrical Conductivity log: The hydraulic complexity of the open borehole conditions is further supported by the electrical conductivity log. Under 'natural' open hole conditions (i.e. no pumping), the salinity along the entire borehole is virtually the same at 0.05–0.06 Sm^{-1}. During the initial pumping stage carried out at 5 m intervals, a constant salinity of about 0.8 sm^{-1} is indicated from 100–300 m. This is followed by an increase to about 0.15 sm^{-1} until 350 m, and a further increase to about 0.25 sm^{-1} to 625 m. At this point there is a sharp decrease to around 0.07 sm^{-1} which stabilises to 800 m followed by a systematic increase to 0.6 sm^{-1} at the borehole bottom. Further pumping at 1 m intervals shows the same patterns but at increased salinities with greatest differences at greatest depths, especially from 700–1,000 m which shows a steady increase from about 0.15–1.2 sm^{-1}.

After a lapse of 3 months the electrical conductivity log was repeated under 'natural' no pumping conditions and indicated dilute water throughout the length of the borehole apart from the deepest part of the borehole. However, during this lapse borehole KLX04 has been subjected to a comprehensive series of hydraulic injection tests and open hole geophysical logging etc. Since the fluid medium used in the hydraulic tests is a dilute water, coupled to the fact that the open borehole is dominated by dilute groundwaters (i.e. residual drilling water plus input of shallow dilute groundwater from the more highly hydraulic conductive sections in the upper part of the borehole), then perhaps it is not surprising that the electrical conductivity measurements without pumping have resulted in a low salinity profile along the borehole. This underlines the necessity of prolonged pumping prior to groundwater sampling.

Hydrochemical logging: Measurement of the borehole was carried out on 2004-07-08, 18 days prior to the differential flow measurements. Compared to the flow measurements, the hydrochemical logging shows a similar range of electrical conductivity values (~ 0.06 Sm^{-1}) from 0–400 m, but these are followed by a higher range (~ 0.1–0.5 Sm^{-1}) from 400–800 m with the same high value at 900 m. This indicates, as inferred above from the flow measurements, that during open hole conditions existing between the hydrochemical logging and the later differential flow measurements, dilute waters have penetrated to a greater depth along the borehole (from about 400–750 m) and the deepest parts of the borehole have become more saline.

The amount of drilling water in the borehole at this stage ranged from 2.31–4.74% from 0–400 m, followed by a sharp increase to a maximum of 54.1% at 735 m, and finally a small decrease to 52.4% at 985 m. The total variation in chloride along the borehole is 27.5–1,510 mg/L, i.e. fresh (0–535 m) to brackish type (535–985 m) groundwater mix.

Comment: The measured high transmissivities relate to the several deformation zones intercepted by KLX04 which, in turn, control the variation in salinity measured under natural and controlled conditions. Due to the high transmissive deformation zones, much of this drilling water mixed with different groundwater sources (mostly from shallow to intermediate depths) have entered the higher transmissive rock mass from the borehole during drilling and subsequently under open hole conditions. These waters will have to be removed initially with great care before 'representative' groundwater can be accessed. Short circuiting therefore may be a major problem.

References: SKB R-06-12, R-06-21, P-05-68, P-05-88, P-04-219.

C2.4.1 KLX04 (0.00–35.00 m; mid. vertical elevation: +6.66 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)			x		
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent			x		
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling			x		
Charge balance ±5% (±10% for <50 mg/L Cl)					
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)			?		

Drilling Water: HLX10 (0–85 m; mid. vertical elevation: –27.86 m). There is no documented sample from the time of drilling (2004-03-13 to 2004-06-28); in the Extended L.2.3 dataset one sample is documented from 2003-03-12 and used here. Na-HCO$_3$ type groundwater with low chloride (6.3 mg/L), δ^{18}O at –10.9‰ VSMOW and δ^{2}H at –78.8‰ V-SMOW; tritium at 7.2 TU, δ^{13}C at –17.45 PDB and ^{14}C at 55.73 pmC.

Charge Balance: Measured Sicada value at +1.05%.

Time Series: Only one sample taken using Tube Sampling in 2004-07-08. Groundwater is fresh (43.6 mg/L Cl) with a drilling water content of 4.75%. Major ions incomplete, no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Incomplete; no carbon isotopes. Tritium at 3.7TU, and $\delta^{18}O$ at –10.5‰ VSMOW.

Trace elements: Lack of data.

General: $Na(Ca)\text{-}HCO_3(Cl)$ fresh groundwater.

Comment: Problem is the absence of time series, drilling water up to 5%, incomplete major ion data, and an absence of trace elements. However, the borehole section is reasonably constrained and the stability of the near-surface groundwater chemistry is more predictable and reflects that expected at these shallow depths. Category 3 allocated.

C2.4.2 KLX04 (104.00–109.00.00 m; mid. vertical elevation: –81.90 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)				x	
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent				x	
Suitable section length				x	
Sampling during drilling				x	
Sampling using PLU hydraulic testing equipment				x	
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)				?	

Drilling Water: HLX10 (0–85 m; mid. vertical elevation: –27.86 m). There is no documented sample from the time of drilling (2004-03-13 to 2004-06-28); in the Extended L.2.3 dataset one sample is documented from 2003-03-12 and used here. $Na\text{-}HCO_3$ type groundwater with low chloride (6.3 mg/L), $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –78.8‰ VSMOW; tritium at 7.2 TU, $\delta^{13}C$ at –17.45‰ PDB and ^{14}C at 55.73 pmC.

Charge Balance: Measured Sicada value at –3.24%.

Time Series: Only one sample taken using PLU hydraulic testing equipment during drilling in 2004-09-30. Groundwater is fresh (23.5 mg/L Cl) with a drilling water content of 0.09%. Major ions complete apart from no TOC.

Isotopes: Incomplete; no carbon isotopes. Tritium at 5.4 TU and $\delta^{18}O$ at –10.3‰ VSMOW.

Trace elements: Lack of data.

General: $Na(Ca)\text{-}HCO_3$ fresh groundwater with a typical recharge signature.

Comment: Major problem is the absence of time series and the deeper level of this sample compared with the previous section where the stability of the near-surface groundwater is more easily predictable. Allocated Category 4.

C2.4.3 KLX04 (510.56–515.56 m; mid. vertical elevation: –486.52 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)			x		
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent			x		
Suitable section length			x		
Sampling during drilling			x		
Sampling using PLU hydraulic testing equipment			x		
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HLX10 (0–85 m; mid. vertical elevation: –27.86 m). There is no documented sample from the time of drilling (2004-03-13 to 2004-06-28); in the Extended L.2.3 dataset one sample is documented from 2003-03-12 and used here. Na-HCO_3 type groundwater with low chloride (6.3 mg/L), $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –78.8‰ VSMOW; tritium at 7.2 TU, $\delta^{13}C$ at –17.45‰ PDB and ^{14}C at 55.73 pmC.

Charge Balance: Measured Sicada value at –2.65%.

Time Series: Only one sample taken using PLU hydraulic testing equipment during drilling in 2004-09-29. Groundwater is brackish (1,480 mg/L Cl) with a drilling water content of 4.41%. Major ions complete.

Isotopes: Incomplete isotopes; no $\delta^{13}C$; ^{14}C at 43.29 pmC. Tritium at 1.2 TU, and $\delta^{18}O$ at –15.1‰ WSMOW indicates a significant glacia component.

Trace elements: Good coverage.

General: Na(Ca)-Cl(SO_4) brackish glacial groundwater.

Comment: Groundwater type often characteristic of this depth. Good coverage of major ions and trace elements, but absence of time series and the presence of 1–5% drilling water. Nevertheless, considered representative for this depth interval and allocated Category 3.

C2.4.4 KLX04 (507.00–530.00 m; mid. vertical elevation: –491.94 m)

Cored Borehole Category	1	2	3	5
Drilling water (≤ 1%)				
Drilling water (≤ 5%)				x
Drilling water (≤ 10%)				
Drilling water (> 10%)				
Time series (adequate)				
Time series (inadequate)				
Time series absent				x
Suitable section length				
Tube sampling				
Sampling using PLU hydraulic testing equipment				
Charge balance ±5% (±10% for <50 mg/L Cl)				x
Major ions (complete)				x
Major ions (incomplete)				
Environmental isotopes (complete)				x
Environmental isotopes (incomplete)				
Monitoring borehole section				x
Hydraulic effects (short circuiting)				x?

Drilling Water: HLX10 (0–85 m; mid. vertical elevation: –27.86 m). There is no documented sample from the time of drilling (2004-03-13 to 2004-06-28); in the Extended L.2.3 dataset one sample is documented from 2003-03-12 and used here. Na-HCO_3 type groundwater with low chloride (6.3 mg/L), $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –78.8‰ VSMOW; tritium at 7.2 TU, $\delta^{13}C$ at –17.45‰ PDB and ^{14}C at 55.73 pmC.

Charge Balance: Measured Sicada value at –1.71%.

Time Series: Monitoring borehole section with sampling limited to one occasion in 2006-11-14. Groundwater is brackish (873 mg/L Cl) with drilling water at 2.27%. Major ions complete.

Isotopes: Complete isotopes; $\delta^{13}C$ at –17.14‰ PDB; ^{14}C at 55.31pmC. Tritium at 1.6 TU, and $\delta^{18}O$ at –13.1‰ VSMOW indicates a cold glacial signature.

Trace elements: Good coverage.

General: Na(Ca)-Cl(HCO_3,SO_4) brackish glacial groundwater.

Comment: Absence of time series is problematic, although an indication of representativity at this level can be obtained by comparing the composition of this sample (873 mg/L Cl) with the section sampled earlier in 2004 and described above (1,480 mg/L Cl) at almost the same depth (–486.52 m elevation). Note the difference also in the $\delta^{18}O$ values, i.e. more enriched at –13.1‰ VSMOW compared to –15.1‰ VSMOW in the preceding sample. There is little doubt that the present sample is not representative and that this is a consequence of borehole activities carried out between the two sampling occasions. Furthermore, this monitoring borehole section is longer (23 m) compared to the earlier section sampled (5 m), which may have facilitated mixing/short circuiting. Allocated Category 5.

C2.4.5 KLX04 (870.00–897.00 m; mid. vertical elevation: –854.86 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					x
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					x
Tube sampling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					x
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX10 (0–85 m; mid. vertical elevation: –27.86 m). There is no documented sample from the time of drilling (2004-03-13 to 2004-06-28); in the Extended L.2.3 dataset one sample is documented from 2003-03-12 and used here. Na-HCO_3 type groundwater with low chloride (6.3 mg/L), $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –78.8‰ VSMOW; tritium at 7.2 TU, $\delta^{13}C$ at –17.45‰ PDB and ^{14}C at 55.73 pmC.

Charge Balance: Measured Sicada value at –2.18%.

Time Series: Monitoring borehole section with sampling limited to one occasion in 2006-11-14. Groundwater is brackish (3,070 mg/L Cl) with drilling water at 2.78%. Major ions incomplete; no Fe(tot), Fe^{2+}, S^{2-}, I and TOC/DOC.

Isotopes: Incomplete isotopes; no carbon isotopes. Tritium at 2.8 TU, and $\delta^{18}O$ at –13.4‰ VSMOW indicates a glacial signature.

Trace elements: Lack of data.

General: Na(Ca)-Cl(SO_4) brackish glacial groundwater.

General: Inadequate time series; at these depths a greater salinity would have been expected and short circuiting to shallower depths is likely, facilitated by the long borehole section sampled (27 m). This would also explain the persistence of depleted $\delta^{18}O$ at –13.4‰ VSMOW and also the tritium signature, although there is the possibility that this tritium may be due to contamination. This section has also been used for hydraulic tests using uranine from 2005-12-08 to 2005-12-15, and residual uranine in and around the borehole section may explain the 2.78% drilling water component. Allocated a Category 5.

C2.4.6 KLX04 (885.00–935.00 m; mid. vertical elevation: –881.16 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					x
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					
Sampling during drilling					x
Sampling using PLU hydraulic testing equipment					x
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX10 (0–85 m; mid. vertical elevation: –27.86 m). There is no documented sample from the time of drilling (2004-03-13 to 2004-06-28); in the Extended L.2.3 dataset one sample is documented from 2003-03-12 and used here. Na-HCO_3 type groundwater with low chloride (6.3 mg/L), $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –78.8‰ VSMOW; tritium at 7.2 TU, $\delta^{13}C$ at –17.45‰ PDB and ^{14}C at 55.73 pmC.

Charge Balance: Sicada value at –2.35%.

Time Series: Only one sample taken using PLU hydraulic testing equipment following drilling in 2004-07-08. Groundwater is brackish (1,510 mg/L Cl) with a drilling water content of 52.40%. Incomplete major ions, no Fe(tot), Fe^{2+}, S^{2-}, I and TOC/DOC.

Isotopes: Incomplete isotopes; no carbon isotopes. Tritium at 2.1 TU, and $\delta^{18}O$ at –13.1‰ VSMOW indicates a weak glacial component.

Trace elements: Lack of data.

General: Na(Ca)-Cl (SO_4) brackish glacial type groundwater

Comment: The groundwater sampled is not characteristic of these depths. This observation, together with absent time series and very high drilling water, suggest short circuiting and mixing from shallower levels, possibly facilitated by the long borehole section (50 m). Allocated Category 5.

C2.4.7 KLX04 (971.21–976.21 m; mid. vertical elevation: –944.38 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)			x		
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent			x		
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment			x		
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)			x		
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HLX10 (0–85 m; mid. vertical elevation: –27.86 m). There is no documented sample from the time of drilling (2004-03-13 to 2004-06-28); in the Extended L.2.3 dataset one sample is documented from 2003-03-12 and used here. Na-HCO_3 type groundwater with low chloride (6.3 mg/L), δ^{18}O at –10.9‰ VSMOW and δ^{2}H at –78.8‰ VSMOW; tritium at 7.2 TU, δ^{13}C at –17.45‰ PDB and ^{14}C at 55.73 pmC.

Charge Balance: Measured Sicada value at –3.30%.

Time Series: Only one sample taken using PLU hydraulic testing equipment following drilling in 2004-09-16. Groundwater is brackish (7,910 mg/L Cl) with a drilling water content of 3.98%. Major ions complete.

Isotopes: Complete isotopes; no carbon isotopes (lack of HCO_3 < 10 mg/L). Tritium below detection (< 0.8TU), and δ^{18}O at –13.8‰ VSMOW indicates a glacial component.

Trace elements: Good coverage.

General: Ca(Na)-Cl(SO_4) brackish glacial groundwater.

Comment: Good coverage of major ions and trace elements, but absence of time series and up to 3.98% drilling water relegates the sample to a Category 3.

Obs. *The presence of brackish glacial groundwaters at these depths, the only locality that they have been found, has been a point of discussion (see SKB R-08-93). Their presence may be linked with the steeply dipping major deformation zone ZMNW929A which intersects borehole KLX04 at 873–973 m.*

KLX04: Tube samples sampled every 50 m from 85.00–935.00 m (2004-07-08) are considered unrepresentative and allocated Category 5.

C2.5 Description of Borehole KLX05

Borehole KLX05 is 1,000.16 m long (vertical depth of 900.89 m), cased to 75.1 m, and inclined at –65.21° from the horizontal. The borehole was drilled from 2004-10-01 to 2005-01-22 to obtain geological information at depth in the south-central part of the Laxemar subarea and to facilitate hydrogeological and hydrochemical investigations at depth. Borehole KLX05 penetrates a relatively heterogeneous rock mass dominated by a mixture of Ävrö granite, fine-grained granite, granite and diorite/gabbro in the upper 400–450 m, followed by mainly quartz monzodiorite with subsidiary zones of fine-grained granite down to the bottom of the borehole. Several zones of deformation occur in the upper 600 m of the bedrock.

Differential Flow Log: Measurements in borehole KLX05, carried out from 2005-04-12 to 2005-04-26, reveal high transmissivities from 100–260 m depth ($10^{5.5}$–10^{6} m^2s^{-1}) with the maximum at 110–130 m. From 260–900 m transmissivities range from below detection (10^{9} m^2s^{-1}) to 10^{8} m^2s^{-1}. Under 'natural conditions' (i.e. no pumping) the groundwater flow is mainly from the borehole to the surrounding bedrock with a maximum measured flow rate of about 10^{3} mL h^{-1} at the area of greatest transmissivity (110–150 m). However, there is some flow into the open borehole at 240–260 m with at a rate of 10^{1}–10^{2} mL h^{-1}. With pumping, all groundwater flow is from the bedrock to the borehole, the variation in groundwater flow rates (10^{1}–$10^{5.1}$ mL h^{-1}) closely reflecting the variation of transmissivity in the surrounding bedrock.

Slightly higher hydraulic conductivity values are reported from the injection tests when compared to the differential flow measurements.

The differential flow results suggest that during open borehole conditions, the groundwater will preferentially move into the surrounding bedrock in the upper 110–150 m. With pumping, for example during sampling, this water will first have to be removed before 'representative' groundwater can be accessed.

Electrical Conductivity log: The hydraulic complexity of the open borehole conditions is further supported by the electric conductivity log. Under 'natural' open hole conditions (i.e. no pumping), the salinity shows a small, but systematic increase from 0.1 Sm^{-1} at 100 m to 0.2 Sm^{-1} at 840 m. At this length, there is a small increase to about 0.28 Sm^{-1} which continues to the bottom of the borehole. During the pumping stage there is an increase in salinity to 0.25 Sm^{-1} at 120 m which continues with a small decrease to 0.2 Sm^{-1} at 600 m. Beyond this point at greater depth there is an increase to 0.4 Sm^{-1} at 610 m followed by a small systematic decrease to just under 0.2 Sm^{-1} at the bottom of the borehole. The overall increase in salinity during pumping is not very marked but time series data from fracture specific water shows strong increases to values of 0.5.5 Sm^{-1} (300 m), 1.7 Sm^{-1} (615 m) and 1.4 Sm^{-1} (795 m).

Hydrochemical logging: Measurement of the borehole was carried out on 2004-07-08, some 9 months prior to the differential flow measurements. This showed the electrical conductivity steadily increasing along the length of the borehole from about 0.08 Sm^{-1} at 40 m to 0.26 Sm^{-1} at 990 m. Compared to the differential flow measurements, the hydrochemical logging generally shows a similar range of electrical conductivity values under open hole conditions.

The amount of drilling water in the borehole at this stage ranged from 2.17–3.65% from 0–440 m, followed by a gradual increase to 24.4% at 800 m followed by a maximum of 66.5% at 940 m. The total variation in chloride along the borehole is 97.9–721 mg/L, i.e. fresh (0–200 m) to brackish (200–940 m) type groundwater mix.

Comment: The measured high transmissivities relate to the several deformation zones intercepted by KLX05 which, in turn, control the variation in salinity measured under natural and controlled conditions. Due to the high transmissive deformation zones, much of this drilling water mixed with different groundwater sources (mostly from shallow to intermediate depths) have entered the higher transmissive rock mass from the borehole during drilling and subsequently under open hole conditions. These waters will first have to be removed with great care before 'representative' groundwater can be accessed. Short circuiting therefore may be a major problem.

References: SKB R-06-12, R-06-21, P-05-160, P-05-195, P-06-233.

C2.5.1 KLX05 (107.80–202.94 m; mid. vertical elevation: –121.90 m)

Cored Borehole					
Category	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					x
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					
Sampling during drilling					x
Sampling using PLU hydraulic testing equipment					x
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX10 (3–85 m; mid. vertical elevation: –29.25 m). There is one sample from the time of drilling borehole KLX05 (2004-10-01 to 2005-01-22); in the Extended L.2.3 dataset this sample is documented from 2005-02-01 and used here. Na-HCO$_3$ type groundwater with low chloride (29.1 mg/L), δ^{18}O at –10.9‰ VSMOW and δ^{2}H at –75.0‰ VSMOW; tritium at 5.2 TU, δ^{13}C at –16.43‰ PDB and ^{14}C at 52.73 pmC.

Charge Balance: Measured Sicada value at –1.32%.

Time Series: Only one sample taken using PLU hydraulic testing equipment during drilling in 2004-10-16. Groundwater is fresh (45.7 mg/L Cl) with a drilling water content of 16.20%. Major ions incomplete; no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Complete; δ^{13}C at –14.29‰ PDB, ^{14}C at 62.56 pmC. Tritium below detection (< 0.8 TU) and δ^{18}O at –10.6‰ VSMOW.

Trace elements: Lack of data.

General: Na-HCO$_3$ fresh groundwater.

General: Problems include a lack of time series, drilling water up to 16.20%, incomplete major ion data, and an absence of trace elements. In addition, the presence of a long borehole section (95.14 m) may facilitate mixing/short circuiting. Allocated Category 5.

C2.5.2 KLX05 (241.00–255.00 m; mid. vertical elevation: –204.84 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)		x			
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)		x			
Time series (inadequate)					
Time series absent					
Suitable section length		x			
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)		x			
Major ions (complete)		x			
Major ions (incomplete)					
Environmental isotopes (complete)		x			
Environmental isotopes (incomplete)					
Monitoring borehole section		x			
Hydraulic effects (short circuiting)		x?			

Drilling Water: HLX10 (3–85 m; mid. vertical elevation: –29.25 m). There is one sample from the time of drilling borehole KLX05 (2004-10-01 to 2005-01-22); in the Extended L.2.3 dataset this sample is documented from 2005-02-01 and used here. Na-HCO_3 type groundwater with low chloride (29.1 mg/L), $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –75.0‰ VSMOW; tritium at 5.2 TU, $\delta^{13}C$ at –16.43‰ PDB and ^{14}C at 52.73 pmC.

Charge Balance: Measured Sicada values at –1.33% to –0.65%.

Time Series: Monitoring borehole section with sampling limited to three occasions in 2006-10-24, 2007-06-19 and 2007-08-14. Reasonable stability but with a small decrease in salinity during the three occasions (626–592 mg/L Cl), reflected by small decreases in Na and SO_4 and a corresponding increase in HCO_3. A sharp increase in drilling water during the second sampling (0.99–11.39%) subsequently deceasing to 2.49% in the last sampling, is observed. Major ions complete for the last sampling in 2007-08-14; otherwise Fe(tot) and Fe^{2+} and TOC/DOC are missing.

Isotopes: Complete for the first and last sampling campaigns; $\delta^{13}C$ at –15.60 to –14.29‰ PDB, ^{14}C at 29.28–30.10 pmC. Tritium below detection (< 0.8TU) and $\delta^{18}O$ at –12.0 to –12.1‰ VSMOW.

Trace elements: Good coverage.

General: Na(Ca)-Cl (HCO_3,SO_4) brackish groundwater of non-marine origin.

Comment: Time series data are few but stable over a time period of 2 months between the second and last sampling campaign; high drilling water reflects the anthropogenic injection of uranine during tracer testing in 2006-12-06 and 2006-12-13, which means that only the first drilling water value (0.99%) is representative. Complete major ion and trace element data. However, the long borehole section (95 m) may have facilitated some groundwater short circuiting/mixing from different sources. The groundwater from the last sampled occasion is selected as most representative assuming < 1% drilling water corresponding to the initial value recorded in 2006. Allocated Category 2.

C2.5.3 KLX05 (625.00–633.00 m; mid. vertical elevation: –549.56 m)

Cored Borehole **Category**	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)					
Drilling water (≤ 5%)			x		
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent			x		
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)			x		
Environmental isotopes (incomplete)					
Monitoring borehole section			x		
Hydraulic effects (short circuiting)					

Drilling Water: HLX10 (3–85 m; mid. vertical elevation: –29.25 m). There is one sample from the time of drilling borehole KLX05 (2004-10-01 to 2005-01-22); in the Extended L.2.3 dataset this sample is documented from 2005-02-01 and used here. Na-HCO_3 type groundwater with low chloride (29.1 mg/L), $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –75.0‰ VSMOW; tritium at 5.2 TU, $\delta^{13}C$ at –16.43‰ PDB and ^{14}C at 52.73 pmC.

Charge Balance: Measured Sicada value at +2.09%.

Time Series: Monitoring borehole section with sampling limited to one occasion in 2006-12-05; salinity of 5,690 mg/L Cl and a drilling water content of 7.31%. Major ions incomplete; no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Complete; no carbon isotopes (lack of HCO_3 at 11.6 mg/L). Tritium below detection (< 0.8TU), and $\delta^{18}O$ at –12.2‰ VSMOW possibly indicates a weak glacial component.

Trace elements: Lack of data.

General: Na(Ca)-Cl(SO_4) brackish non-marine groundwater (possibly with a weak glacial component).

Comment: Inadequate time series and high drilling water content, but overall the composition expected for this depth and therefore important for repository level information. Allocated Category 3.

C2.6 Description of Borehole KLX06

Borehole KLX06 is 994.94 m long (vertical depth of 805.67 m), cased to 100.30 m, and inclined at –65.19° from the horizontal, was drilled between 2004-08-25 to 2004-11-25. The borehole was drilled to obtain geological information of the northern part of the Laxemar subarea, especially the large Mederhult defomation zone (ZSMEW002A). The main rock type intercepted by the borehole is Avrö granite with frequent horizons mainly of granite but also some fine-grained granite. The average fracture frequency for the borehole length is 0.5 fractures m^{-1} with increases between 200–260 m and 300–390 m characterised by intense alteration. This latter section, which shows a strong foliation in places and also some laumontite alteration, is interpreted to be the Mederhult deformation zone.

Differential Flow Log: Measurements in borehole KLX06 carried out from 2005-02-08 to 2005-03-01 reveal high transmissivities from 100–380 m depth (10^{6}–$10^{4.5}$ m^2s^{-1}); isolated highs occur associated with single fractures/zones at 565 m ($10^{5.3}$ m^2s^{-1}) and 780 m (10^{6} m^2s^{-1}). The remaining borehole length from 380 m to the borehole bottom shows a sharp decrease in transmissivity to average values of 10^{8}–10^{7} m^2s^{-1}. Under 'natural conditions' (i.e. no pumping) the groundwater flow at 100–400 m is from the surrounding bedrock into the borehole with a maximum measured flow rate of 10^{5}–$10^{5.2}$ mL h^{-1}; from 400 m to the borehole bottom the natural flow is reversed towards the host bedrock with average rates of 10^{2}–10^{3} mL h^{-1} apart from the two isolated high transmissive locations which record 10^{4} and 10^{5} mL h^{-1} respectively. With pumping, all the groundwater flow is towards the borehole. Hydraulic injection tests have been conducted with the purpose of describe the rock hydraulic parameters (mainly transmissivity) and to collect groundwater samples for analysis at specific depths. The transmissivity measurements were in general agreement with the differential flow log interpretations.

The above flow log measurements suggest that during open borehole conditions the groundwater will preferentially move into the surrounding bedrock in the upper 100–380 m. This water will have to be removed initially before 'representative' groundwater can be accessed.

Electrical Conductivity log: The hydraulic complexity of the open borehole conditions is further supported by the electrical conductivity log. Under 'natural' open hole conditions (i.e. no pumping), the salinity shows a small, but systematic increase from just under 0.05 Sm^{-1} at 100 m to 0.09 Sm^{-1} at 980 m; one small 'kink' occurs in the profile at 390 m, i.e. the transition to the less transmissive borehole length. During the pumping stage there is a general increase in the salinity profile from 0.05 Sm^{-1} at 100 m to 0.15 Sm^{-1} at 780 m; this increases to 0.3 Sm^{-1} at 815 m and continues to the bottom of the borehole.

Hydrochemical logging: Measurement of the borehole was carried out on 2004-12-21 almost 3 months prior to the differential flow measurements. The electrical conductivity show a small but steady increase along the length of the borehole from about 0.05 Sm^{-1} at 40 m to 0.07 Sm^{-1} at 840 m, followed by a sharp increase to 0.19 Sm^{-1} at 940 m. Compared to the flow measurements, the hydrochemical logging generally shows a similar range of electrical conductivity values under open hole conditions.

The amount of drilling water in the borehole at this stage ranged from 7.5–9.6% from 0–240 m, 14.4–23.9% from 240–540 m, a peak of 50% at 640 m followed by a decrease to 37% from 640–840 m, and finally to a maximum value of 64% at 940 m. The total variation in chloride along the borehole is 29.5–429 mg/L Cl, i.e. fresh (0–840 m) to brackish type (840–940 m) groundwater mix.

Comment: The measured high transmissivities relate to the several deformation zones intercepted by KLX06 which, in turn, control the variation in salinity measured under natural and controlled conditions. Due to the high transmissive deformation zones, much of this drilling water mixed with different groundwater sources (mostly from shallow to intermediate depths) have entered the higher transmissive rock mass from the borehole during drilling and subsequently under open hole conditions. These waters will first have to be removed with great care before 'representative' groundwater can be accessed. Short circuiting therefore may be a major problem.

References: SKB R-06-12, R-06-21, P-05-74, P-05-85, P-05-184, P-05-244.

C2.6.1 KLX06 (0–40.00 m; mid. vertical elevation: –0.48 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)			x		
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent			x		
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling			x		
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)			x?		

Drilling Water: HLX20 (9.10–202.00 m; mid. vertical elevation: –80.67 m). There is no documented sample from the time of drilling (2004-08-25 to 2004-11-25) in the Extended L.2.3 dataset; the closest sample is documented from 2004-06-24 and therefore used here. Na-HCO_3 type groundwater with low chloride (29.4 mg/L), $\delta^{18}O$ at –11.3‰ VSMOW and δ^2H at –80.3‰ VSMOW; tritium is below detection (< 0.8TU), $\delta^{13}C$ at –17.01‰ PDB and ^{14}C at 41.68 pmC.

Charge Balance: Measured Sicada value at +5.33% (< ±10%).

Time Series: Only one sample taken using tube sampling in 2004-12-21. Groundwater is fresh (42.90 mg/L Cl) with a drilling water content of 8.05%. Major ions incomplete, no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Incomplete; no carbon isotopes. Tritium at 4.6 TU and $\delta^{18}O$ at –10.5‰ VSMOW.

Trace elements: Lack of data.

General: Na(Ca)-HCO_3 fresh groundwater with a shallow bedrock recharge signature.

Comment: Problem is an absence of time series, drilling water up to 8%, incomplete major ion data, and an absence of trace elements. However, the stability of the near-surface groundwater chemistry is more predictable and reflects that expected at these shallow depths. Allocated Category 3.

C2.6.2 KLX06 (103.00–202.26 m; mid. vertical elevation: –120.23 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					x
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					
Sampling during drilling					x
Sampling using PLU hydraulic testing equipment					x
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX20 (9.10–202.00 m; mid. vertical elevation: –80.67 m). There is no documented sample from the time of drilling (2004-08-25 to 2004-11-25) in the Extended L.2.3 dataset; the closest sample is documented from 2004-06-24 and therefore used here. Na-HCO$_3$ type groundwater with low chloride (29.4 mg/L), δ^{18}O at –11.3‰ VSMOW and δ^{2}H at –80.3‰ VSMOW; tritium is below detection (< 0.8TU), δ^{13}C at –17.01‰ PDB and ^{14}C at 41.68 pmC.

Charge Balance: Measured Sicada value at +2.2%.

Time Series: Only one sample taken using PLU hydraulic testing equipment during drilling in 2004-09-05. Groundwater is fresh (25.4 mg/L Cl) with a drilling water content of 17.40%. Major ions incomplete; no Fe(tot), Fe(II), S^{2-}, and TOC/DOC.

Isotopes: Complete; δ^{13}C at –16.23 PDB, ^{14}C at 48.15 pmC. Tritium at 2.8 TU and δ^{18}O at –11.3‰ VSMOW.

Trace elements: Lack of data.

General: Na-HCO$_3$ fresh groundwater with a shallow recharge signature.

General: Problem is a lack of time series, drilling water up to 17.40%, incomplete major ion data and an absence of trace elements. In addition, a long borehole section (99 m) which may have facilitated short circuiting and mixing. Allocated Category 5.

C2.6.3 KLX06 (260.50–268.70 m; mid. vertical elevation: –220.38 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					x
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					x
Sampling during drilling					x
Sampling using PLU hydraulic testing equipment					x
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HLX20 (9.10–202.00 m; mid. vertical elevation: –80.67 m). There is no documented sample from the time of drilling (2004-08-25 to 2004-11-25) in the Extended L.2.3 dataset; the closest sample is documented from 2004-06-24 and therefore used here. Na-HCO_3 type groundwater with low chloride (29.4 mg/L), $\delta^{18}O$ at –11.3‰ VSMOW and $\delta^{2}H$ at –80.3‰ VSMOW; tritium is below detection (< 0.8TU), $\delta^{13}C$ at –17.01‰ PDB and ^{14}C at 41.68 pmC.

Charge Balance: Measured Sicada value at –2.06%.

Time Series: Only one sample taken using PLU hydraulic testing equipment during drilling in 2004-09-11. Groundwater is fresh (15.7 mg/L Cl) with a drilling water content of 4.03%. Major ions incomplete; no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Complete; $\delta^{13}C$ at –16.31‰ PDB, ^{14}C at 47.29 pmC. Tritium at 1.5 TU and $\delta^{18}O$ at –11.2‰ VSMOW.

Trace elements: Lack of data.

General: Na-HCO_3 fresh groundwater with a shallow recharge signature.

Comment: Little difference from the preceding borehole section despite the increase in depth. Major problem is a lack of time series, incomplete major ion data and suspected disturbances connected with the drilling (e.g. drilling water at 4.03%). Allocated Category 5.

C2.6.4 KLX06 (260.00–265.00 m; mid. vertical elevation: –218.51 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)			x		
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent			x		
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment			x		
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section					
Hydraulic effects (short circuiting)			x?		

Drilling Water: HLX20 (9.10–202.00 m; mid. vertical elevation: –80.67 m). There is no documented sample from the time of drilling (2004-08-25 to 2004-11-25) in the Extended L.2.3 dataset; the closest sample is documented from 2004-06-24 and therefore used here. Na-HCO_3 type groundwater with low chloride (29.4 mg/L), $\delta^{18}O$ at –11.3‰ VSMOW and $\delta^{2}H$ at –80.3‰ VSMOW; tritium is below detection (< 0.8TU), $\delta^{13}C$ at –17.01‰ PDB and ^{14}C at 41.68 pmC.

Charge Balance: Measured Sicada value at –2.99%.

Time Series: One sample taken using PLU hydraulic testing equipment in 2005-03-09; this is virtually the same position as the preceding sample documented as sampling during drilling. Groundwater is fresh (36.8 mg/L Cl) with a drilling water content of 5.68%. Major ions complete apart from DOC.

Isotopes: Incomplete; no carbon isotopes. Tritium below detection (< 0.8TU) and $\delta^{18}O$ at –11.1‰ VSMOW.

Trace elements: Lack of data.

General: Na-HCO_3 fresh groundwater with a shallow bedrock signature.

General: Little difference from the preceding borehole section; improvement due to an additional sample following a break of almost 6 months and an absence of tritium. However, drilling water still significant at 5.68% (small increase) together with incomplete major ion data and an absence of trace elements. However, sufficient additional data to allocate a Category 3.

C2.6.5 KLX06 (256.00–275.00 m; mid. vertical elevation: –221.18 m)

Cored Borehole **Category**	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)					
Drilling water (≤ 5%)			x		
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)			x		
Time series absent					
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section			x		
Hydraulic effects (short circuiting)					

Drilling Water: HLX20 (9.10–202.00 m; mid. vertical elevation: –80.67 m). There is no documented sample from the time of drilling (2004-08-25 to 2004-11-25) in the Extended L.2.3 dataset; the closest sample is documented from 2004-06-24 and therefore used here. Na-HCO_3 type groundwater with low chloride (29.4 mg/L), $\delta^{18}O$ at –11.3‰ VSMOW and $\delta^{2}H$ at –80.3‰ VSMOW; tritium is below detection (< 0.8TU), $\delta^{13}C$ at –17.01‰ PDB and ^{14}C at 41.68 pmC.

Charge Balance: Measured Sicada values at –1.95% to –0.79%.

Time Series: Monitoring borehole section sampled on two occasions; 2006-07-04 and 2006-10-24. This section is similar, but not identical, to the two preceding samples taken with the PLU equipment in 2004 and 2005. Groundwater is fresh (~ 58 mg/L Cl) with a drilling water content of 3.56–3.62%. Complete major ions.

Isotopes: Complete; $\delta^{13}C$ at –16.47‰ PDB, ^{14}C at 35.62 pmC. Tritium below detection (< 0.8TU) and $\delta^{18}O$ at –11.3‰ VSMOW.

Trace elements: Good coverage.

General: Na-HCO_3 fresh groundwater with a typical shallow recharge signature. Little difference from the preceding borehole sections at this location. Problem is the monitoring section sampling protocol (i.e. lack of time series to check stability during sampling). Allocated Category 3.

C2.6.6 KLX06 (554.00–570.00 m; mid. vertical elevation: –475.27 m)

Cored Borehole					
Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)			?		
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)			x		
Time series absent					
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)			x		
Environmental isotopes (incomplete)					
Monitoring borehole section			x		
Hydraulic effects (short circuiting)					

Drilling Water: HLX20 (9.10–202.00 m; mid. vertical elevation: –80.67 m). There is no documented sample from the time of drilling (2004-08-25 to 2004-11-25) in the Extended L.2.3 dataset; the closest sample is documented from 2004-06-24 and therefore used here. Na-HCO_3 type groundwater with low chloride (29.4 mg/L), $\delta^{18}O$ at –11.3‰ VSMOW and $\delta^{2}H$ at –80.3‰ VSMOW; tritium is below detection (< 0.8TU), $\delta^{13}C$ at –17.01‰ PDB and ^{14}C at 41.68 pmC.

Charge Balance: Measured Sicada values at –0.08% to +0.40%.

Time Series: Monitoring borehole section sampled on two occasions; 2006-07-04 and 2006-10-24. Groundwater is brackish (~ 778–878 mg/L Cl) with a drilling water content of 9.31–10.30%. Major ions complete.

Isotopes: Complete; $\delta^{13}C$ at –18.84‰ PDB, ^{14}C at 37.61 pmC. Tritium below detection (< 0.8TU) and $\delta^{18}O$ at –13.0‰ VSMOW indicating a glacial component.

Trace elements: Good coverage.

General: Na(Ca)-Cl(SO_4) brackish glacial groundwater.

Comment: Groundwater typical of this depth. Major problem is the monitoring section sampling protocol with inadequate time series to check stability during sampling. Furthermore, this section has been subject to hydraulic flow tests in 2005-11-23 to 2005-11-28 using uranine as a tracer. When later sampling has been conducted, residual uranine may have contributed to an erroneously calculated drilling water content. This would explain the high drilling water contents sampled in this case. These above uncertainties restrict this sample to a Category 3.

C2.6.7 KLX06 (558.20–563.20 m; mid. vertical elevation: –474.21 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					x
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					x
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					x
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX20 (9.10–202.00 m; mid. vertical elevation: –80.67 m). There is no documented sample from the time of drilling (2004-08-25 to 2004-11-25) in the Extended L.2.3 dataset; the closest sample is documented from 2004-06-24 and therefore used here. Na-HCO_3 type groundwater with low chloride (29.4 mg/L), $\delta^{18}O$ at –11.3‰ VSMOW and $\delta^{2}H$ at –80.3‰ VSMOW; tritium is below detection (< 0.8TU), $\delta^{13}C$ at –17.01‰ PDB and ^{14}C at 41.68 pmC.

Charge Balance: Measured Sicada value at –1.45%.

Time Series: Only one sample taken using PLU hydraulic testing equipment in 2005-03-16. Groundwater is brackish (348 mg/L Cl) with a drilling water content of 21.40%. Major ions incomplete; no Fe(tot), Fe^{2+}, S^{2-} and TOC/ DOC.

Isotopes: Incomplete; no carbon isotopes. Tritium close to detection at 1.0 TU and $\delta^{18}O$ at –11.8‰ VSMOW.

Trace elements: Lack of data.

General: Na-Cl (SO_4,HCO_3) brackish groundwater of mixed origin.

Comment: Problem is a lack of time series, drilling water at 21.40%, incomplete major ion and isotope data and an absence of trace elements. Groundwater composition is not representative for this depth range. Allocated Category 5.

C2.6.8 KLX06 (715.14–784.94 m; mid. vertical elevation: –621.86 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					x
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					
Sampling during drilling					x
Sampling using PLU hydraulic testing equipment					x
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX20 (9.10–202.00 m; mid. vertical elevation: –80.67 m). There is no documented sample from the time of drilling (2004-08-25 to 2004-11-25) in the Extended L.2.3 dataset; the closest sample is documented from 2004-06-24 and therefore used here. Na-HCO_3 type groundwater with low chloride (29.4 mg/L), $\delta^{18}O$ at –11.3‰ VSMOW and $\delta^{2}H$ at –80.3‰ VSMOW; tritium is below detection (< 0.8TU), $\delta^{13}C$ at –17.01‰ PDB and ^{14}C at 41.68 pmC.

Charge Balance: Measured Sicada value at –0.70%.

Time Series: Only one sample taken using PLU hydraulic testing equipment during drilling in 2004-10-29. Groundwater is brackish (1,330 mg/L Cl) with a drilling water content of 48.70%. Major ions incomplete; no Br, Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Lack of data.

Trace elements: Lack of data.

General: Na(Ca)-Cl(SO_4) brackish groundwater of mixed origin.

Comment: Problem is a lack of time series, drilling water at 48.70%, incomplete major ion data and an absence of trace elements and isotopes. In addition, a long borehole section (~ 70 m) which may facilitate mixing/short circuiting of groundwaters from different sources. Allocated Category 5.

C2.6.9 KLX06 (776.20–781.20 m; mid. vertical elevation: –642.90 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					x
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					x
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					x
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HLX20 (9.10–202.00 m; mid. vertical elevation: –80.67 m). There is no documented sample from the time of drilling (2004-08-25 to 2004-11-25) in the Extended L.2.3 dataset; the closest sample is documented from 2004-06-24 and therefore used here. Na-HCO_3 type groundwater with low chloride (29.4 mg/L), $\delta^{18}O$ at –11.3‰ VSMOW and δ^2H at –80.3‰ VSMOW; tritium is below detection (< 0.8TU), $\delta^{13}C$ at –17.01‰ PDB and ^{14}C at 41.68 pmC.

Charge Balance: Measured Sicada value at +0.05%.

Time Series: Only one sample taken using PLU hydraulic testing equipment in 2005-03-23. Groundwater is brackish (1,240 mg/L Cl) with a drilling water content of 23.20%. Major ions incomplete; no Br, Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Incomplete; no carbon isotopes; tritium close to detection at 1.2 TU, and $\delta^{18}O$ at –12.6‰ VSMOW indicates a possible weak glacial component.

Trace elements: Lack of data.

General: Na(Ca)-Cl(SO_4,HCO_3) brackish groundwater of mixed origin including a possible weak glacial component.

General: Problem is a lack of time series, drilling water at 23.20%, incomplete major ion and isotope data and an absence of trace elements. Not considered representative at this depth range. Allocated Category 5.

KLX06: Tube samples sampled every 50 m from 85.00–935.00 m (2004-12-21) are considered unrepresentative and allocated Category 5.

C2.7 Description of Borehole KLX07A

Borehole KLX07A is 844.73 m long (vertical depth of 649.74 m), cased to 100.46 m, and inclined at –60.03° from the horizontal. The borehole was drilled from 2005-01-06 to 2005-05-04 to penetrate the large E-W Deformation Zone (ZSMEW007A) which is located central to the Laxemar subarea. The dominating rock type encountered consists of the Ävrö granite and is characterised by a series of crush zones mainly concentrated at 110–150 m, 350–380 m and from 600–850 m borehole length.

Differential Flow Log: Measurements carried out in borehole KLX07A from 2005-06-09 to 2005-06-29 revealed transmissivities ranging from below detection at 10^{9} m^2s^{-1} to 10^{5} m^2s^{-1}; these values characterise most of the borehole to the maximum borehole depth measured at around 830 m. Higher transmissivities up to $10^{4.7}$ m^2s^{-1} occur from 150–250 m, and horizons of lower transmissivity below 10^{6} m^2s^{-1} occur from approximately 500–750 m and from approximately 770–830 m. Under 'natural conditions' (i.e. no pumping) the groundwater flow is dominantly from the borehole to the surrounding bedrock at 100–310 m and at 620–820 m, in both cases with flow rates ranging from $10^{1.3}$–10^{5} mL h^{-1}; from 340–560 m the natural flow is reversed towards the open borehole with average flow rates of $10^{1.3}$–10^{4} mL h^{-1}. With pumping, all groundwater flow is towards the borehole. Hydraulic injection tests have been conducted with the purpose of describing the rock hydraulic parameters (mainly transmissivity) and to collect groundwater samples for analysis at specific depths. The transmissivity measurements are in general agreement with the differential flow log interpretations.

Electrical Conductivity log: The hydraulic complexity of the open borehole conditions is further supported by the electrical conductivity log. Under 'natural' open hole conditions (i.e. no pumping), a uniform salinity (~ 0.04 Sm^{-1}) is indicated from 100–400 m, followed by a small increase to about 0.05 Sm^{-1} down to around 550 m. At this point a small increase to 0.07 Sm^{-1} occurs, and from thereon a salinity from 0.06–0.07 Sm^{-1} continues to the limit of the measurements at about 840 m. During the pumping stage there is a general increase in the salinity profile to 0.1 Sm^{-1} at 100 m to almost 0.4 Sm^{-1} at 480 m. This is followed by a small decrease to 0.2 Sm^{-1} at 640 m, which then continues to 740 m, whereupon there is a sharp increase to over 1.0 Sm^{-1} which continues to 840 m.

Hydrochemical logging: Measurement of the borehole under open hole conditions was carried out on 2005-06-08, only 4 days prior to the differential flow measurements. This showed a range of electrical conductivity values of 0.04–0.05 Sm^{-1} from 100–500 m before increasing steadily to 0.065 Sm^{-1} at 800 m, i.e. generally similar to the results of the differential flow log.

The amount of drilling water in the borehole at this stage ranged from 2–4% from 100–700 m, followed by a rapid increase to 9% at 800 m. The total variation in chloride along the borehole is 16.40–71.50 mg/L Cl, i.e. fresh groundwater mix.

Comment: The measured high transmissivities relate to the several deformation zones intercepted by KLX07A which, in turn, control the variation in salinity measured under natural and controlled conditions. Due to the high transmissive deformation zones, much of this drilling water mixed with different groundwater sources (mostly from shallow to intermediate depths) have entered the higher transmissive rock mass from the borehole during drilling and subsequently under open hole conditions. These waters will first have to be removed with great care before 'representative' groundwater can be accessed. Short circuiting therefore may be a major problem.

References: SKB P-05-22, P-05-225, P-05-226, P-05-273, P-06-14, P-06-16.

C2.7.1 KLX07A (0–30.00 m; mid. vertical elevation: +5.54 m)

Cored Borehole					
Category	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)					
Drilling water (≤ 5%)				x	
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent				x	
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling				x	
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KLX07A between 2005-01-06 and 2005-05-04, i.e. sample collected in 2005-02-01 and used here. Na-HCO_3 type groundwater with low chloride (29.1 mg/L) and low drilling water content (0.24%), $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –75.0‰ VSMOW; tritium at 5.2 TU, $\delta^{13}C$ at –16.43‰ PDB and ^{14}C at 51.72 pmC.

Charge Balance: Measured Sicada value at +4.06%.

Time Series: Only one sample taken using Tube Sampling in 2005-06-08. Groundwater is fresh (27.4 mg/L Cl) with a drilling water content of 2.21%. Major ions incomplete; no Fe(tot), Fe^{2+}, $S^{2-}$and TOC/DOC.

Isotopes: Lack of data.

Trace elements: Lack of data.

General: Na(Ca)-HCO_3 fresh groundwater of shallow origin.

Comment: Problem is an absence of time series, a drilling water content of 2.21%, incomplete major ion data, and an absence of isotope data and trace elements. However, the borehole section is reasonably constrained and the stability of the near-surface groundwater chemistry is usually more predictable and representative of that expected at these shallow depths. Allocated Category 4.

C2.7.2 KLX07A (103.00–193.00 m; mid. vertical elevation: –100.05 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					x
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					x
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KLX07A between 2005-01-06 and 2005-05-04, i.e. sample collected in 2005-02-01 and used here. Na-HCO_3 type groundwater with low chloride (29.1 mg/L) and low drilling water content (0.24%), $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –75.0‰ VSMOW; tritium at 5.2 TU, $\delta^{13}C$ at –16.43‰ PDB and ^{14}C at 51.72 pmC.

Charge Balance: Measured Sicada value at –0.18%.

Time Series: Only one sample taken using PLU hydraulic testing equipment in 2005-10-31. Groundwater is fresh (45.7 mg/L Cl) with a drilling water content of 0.90%. Major ions incomplete; no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Lack of data.

Trace elements: Lack of data.

General: Na-HCO_3 fresh groundwater of shallow recharge origin.

Comment: Problem is an absence of time series, incomplete major ion data, absence of trace elements and isotopes, and an extra long borehole section (90 m) which may have facilitated mixing/short circuiting. Allocated Category 5.

C2.7.3 KLX07A (193.00–313.00 m; mid. vertical elevation: –178.87 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					x
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					
Tube sampling					
Sampling using PLU hydraulic testing equipment					x
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KLX07A between 2005-01-06 and 2005-05-04, i.e. sample collected in 2005-02-01 and used here. Na-HCO_3 type groundwater with low chloride (29.1 mg/L) and low drilling water content (0.24%), $\delta^{18}O$ at –10.9‰ VSMOW and δ^2H at –75.0‰ VSMOW; tritium at 5.2 TU, $\delta^{13}C$ at –16.43‰ PDB and ^{14}C at 51.72 pmC.

Charge Balance: Measured Sicada value at +0.75%.

Time Series: Only one sample taken using PLU hydraulic testing equipment in 2005-11-15. Groundwater is fresh (98.8 mg/L Cl) with a drilling water content of 2.71%. Major ions incomplete; no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Lack of data.

Trace elements: Lack of data.

General: Na-$HCO_3(Cl,SO_4)$ fresh groundwater of mixed origin.

Comment: Problem is an absence of time series, incomplete major ion data, absence of trace elements and isotopes, and an extra long borehole section (120 m) which may have facilitated mixing/short circuiting. Allocated Category 5.

C2.7.4 KLX07A (335.00–455.00 m; mid. vertical elevation: –283.52 m)

Cored Borehole

Category	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					x
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					x
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KLX07A between 2005-01-06 and 2005-05-04, i.e. sample collected in 2005-02-01 and used here. Na-HCO_3 type groundwater with low chloride (29.1 mg/L) and low drilling water content (0.24%), $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –75.0‰ VSMOW; tritium at 5.2 TU, $\delta^{13}C$ at –16.43‰ PDB and ^{14}C at 51.72 pmC.

Charge Balance: Measured Sicada value at –0.98%.

Time Series: Only one sample taken using PLU hydraulic testing equipment in 2005-11-08. Groundwater is fresh (346.0 mg/L Cl) with a drilling water content of 4.6%. Major ions incomplete; no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Lack of data.

Trace elements: Lack of data.

General: Na-Cl(HCO_3,SO_4) brackish groundwater of mixed origin.

Comment: Problem is a lack of time series, incomplete major ion data, absence of trace elements and isotopes, and an extra long borehole section (120 m) which may have facilitated short circuiting. Allocated Category 5.

C2.7.5 KLX07A (610.00–655.00 m; mid. vertical elevation: –463.62 m)

Cored Borehole					
Category	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					x
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					x
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KLX07A between 2005-01-06 and 2005-05-04, i.e. sample collected in 2005-02-01 and used here. Na-HCO$_3$ type groundwater with low chloride (29.1 mg/L) and low drilling water content (0.24%), δ^{18}O at –10.9‰ VSMOW and δ^{2}H at –75.0‰ VSMOW; tritium at 5.2 TU, δ^{13}C at –16.43‰ PDB and ^{14}C at 51.72 pmC.

Charge Balance: Measured Sicada value at +1.04%.

Time Series: Only one sample taken using PLU hydraulic testing equipment in 2005-12-03. Groundwater is brackish (1,270 mg/L Cl) with a small increase in Mg (16.7 mg/L) and a drilling water content of 10.10%. Major ions incomplete; no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Lack of data.

Trace elements: Lack of data.

General: Na(Ca)-Cl(SO$_4$) brackish groundwater of mixed origin.

Comment: Problem is a lack of time series, incomplete major ion data, absence of trace elements and isotopes, and a 45 m long borehole section (100 m) which may facilitate mixing/short circuiting. Allocated Category 5.

C2.7.6 KLX07A (753.00–780.00 m; mid. vertical elevation: –569.69 m)

Cored Borehole					
Category	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					x
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent					
Suitable section length					
Sampling during sampling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					x
Major ions (incomplete)					
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					
Monitoring borehole section					x
Hydraulic effects (short circuiting)					?

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KLX07A between 2005-01-06 and 2005-05-04, i.e. sample collected in 2005-02-01 and used here. Na-HCO_3 type groundwater with low chloride (29.1 mg/L) and low drilling water content (0.24%), $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –75.0‰ VSMOW; tritium at 5.2 TU, $\delta^{13}C$ at –16.43‰ PDB and ^{14}C at 51.72 pmC.

Charge Balance: Measured Sicada values at –1.70% to +0.76%.

Time Series: Monitoring borehole section with sampling on four occasions over a period of about 1 year (2006-06-20, 2006-12-05, 2007-06-13 and 2007-06-27). Time series show a variation in salinity from 318–1,680 mg/L Cl, with the last sampling occasions (2007-06 13 to 2007-06-27) showing a minor increase from 1,590–1,680 mg/L Cl. This is supported by small increases in Na, Ca, K, Mg (8.0–20.1 mg/L) and SO_4, and a small decrease in HCO_3. The time series also shows a systematic increase in drilling water content from 1.75–5.37% during the total sampling period. Major ions complete except for the second sampling campaign in 2006-12-05 where there are no Fe(tot), Fe^{2+}, S^{2-} or TOC/DOC data.

Isotopes: Complete (apart from the second sampling in 2006-12-05); $\delta^{13}C$ at –17.88 to –19.30‰, ^{14}C at 57.28–53.50 pmC. Tritium variable at 5.20–4.30 TU and $\delta^{18}O$ at –11.6 to –11.0‰ VSMOW.

Trace elements: Good coverage.

General: Na(Ca)-Cl(SO_4) brackish groundwater of a mixed non-marine origin (Mg at 8–21 mg/L) with no distinct cold climate component.

Comment: Inadequate time series shows chemical instability and this is supported by an increase in drilling water, variable tritium and an increasing depletion in δ^{18}O during sampling. Increase in tritium may be due to contamination (see section 3.1.1).

This borehole section was also the location for a series of hydraulic flow tests using uranine as a tracer, two of which may have influenced the last two groundwater sampling occasions. This might explain the increase to 5.25% and 5.37% drilling water from the earlier sampling occasion in 2006-12-05 which recorded 4.01%.

Compared to the next section described below, sampled at an earlier occasion which included the section presently monitored and described here, the composition was approaching that recorded by the last two sampling occasions in the present monitoring section (1,258 vs. 1,590–1,680 mg/L Cl). This may indicate an approach to the true groundwater composition; additional time series are required. However, in general there are still too many uncertainties and therefore the present groundwaters are allocated a Category 5.

C2.7.7 KLX07A 747.00–792.00 m; mid. vertical elevation: –572.06 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					x
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					
Sampling during drilling					
Tube sampling					
Sampling using PLU hydraulic testing equipment					x
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KLX07A between 2005-01-06 and 2005-05-04, i.e. sample collected in 2005-02-01 and used here. Na-HCO_3 type groundwater with low chloride (29.1 mg/L) and low drilling water content (0.24%), δ^{18}O at –10.9‰ VSMOW and δ^{2}H at –75.0‰ VSMOW; tritium at 5.2 TU, δ^{13}C at –16.43‰ PDB and ^{14}C at 51.72 pmC.

Charge Balance: Measured Sicada value at +0.16%.

Time Series: Only one sample taken using PLU hydraulic testing equipment in 2005-11-25. Groundwater is brackish (1,250 mg/L Cl) with a drilling water content of 7.13%. Major ions incomplete, no Br, Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Lack of data.

Trace elements: Lack of data.

General: Na(Ca)-Cl(SO_4) brackish groundwater of mixed origin.

General: Problem is a lack of time series, incomplete major ion data, absence of trace elements and isotopes, and a 45 m long borehole section which may facilitate mixing/short circuiting. Allocated Category 5.

KLX07A: Tube samples sampled every 50 m from 80.00–830.00 m (2005-06-08) are considered unrepresentative and allocated Category 5.

C2.8 Description of Borehole KLX08

Borehole KLX08 (designated chemistry borehole) is 1,000.41 m long (vertical depth of 857.13 m), cased to 100.33 m, and inclined at –60.50° from the horizontal. The borehole was drilled from 2005-04-04 to 2005-06-13 to penetrate the large E-W Deformation Zone (ZSMEW007A) which is located central to the Laxemar subarea. The dominating rock type encountered consists of the Ävrö granite and is characterised by a series of deformation zones mainly concentrated at 100–300 m and 400–500 m with more individual zones at about 770 m and 930 m borehole length. There is a clear correlation between oxidation, both occurrence and intensity, and fracture frequency. The distribution of total fractures in the core is typically in the range of 0–10 fractures m^{-1} with minor sections containing elevated fracture frequencies. Crushed sections notably occur at 120, 150, 220, 300, 410, 650 and 770 m borehole length.

Differential Flow Log: Measurements carried out in borehole KLX08 from 2005-07-26 to 2005-10-18 revealed transmissivities ranging from below detection at 10^{-9} m^2s^{-1} to $10^{-4.9}$ m^2s^{-1}; the high values characterise most of the borehole to about 400 m borehole length whereupon they decrease to about 10^{-9} m^2s^{-1} to 10^{-6} m^2s^{-1} until about 500 m and also between 600–680 m. Outside these borehole lengths at 310–360 m, 500–600 m and below 680 m, only two values could be measured above detection; $10^{-8.7}$ m^2s^{-1} at 770 m and 10^{-7} m^2s^{-1} at 855 m. The greatest transmissivities up to $10^{-4.9}$ m^2s^{-1} occur from 100–200 m and at 400 m, and horizons of lower transmissivity below 10^{-6} m^2s^{-1} occur at approximately 260–300 m 400–7,490 m and from approximately 615–665 m. Under 'natural conditions' (i.e. no pumping) the groundwater flow is dominantly from the borehole to the surrounding bedrock at 160–305 m and at 385–495 m, with flow rates ranging from $10^{1.4}$–$10^{5.7}$ mL h^{-1}; two point sources occur at about 680 m ($10^{1.9}$ mL h^{-1}) and at 855 m ($10^{2.1}$ mL h^{-1}). In contrast, from 100–160 m the flow is towards the open borehole with average flow rates of 10^{1} –$10^{4.8}$ mL h^{-1}. With pumping, all groundwater flow is towards the borehole.

Hydraulic injection tests have been conducted with the purpose of describing the rock hydraulic parameters (mainly transmissivity). The transmissivity measurements are in general agreement with the differential flow log interpretations. Furthermore, the hydraulic injection tests indicated the presence of larger transmissive zones in the vicinity of the borehole which could be caused by steep fractures close to, but not intercepted by the borehole KLX08. These fractures are probably connected to the borehole by lower transmissive fractures.

Electrical Conductivity log: The hydraulic complexity of the open borehole conditions is further supported by the electrical conductivity log. Under 'natural' open hole conditions (i.e. no pumping), a fairly uniform salinity (~ 0.05 Sm^{-1}) is indicated from 100–500 m, followed by a sharp increase between 500–600 m to almost 0.40 Sm^{-1}. This only decreases fractionally to ~ 0.30 Sm^{-1} at 980 m borehole length. During the pumping stage there is a general increase in the salinity profile to 0.06 Sm^{-1} at 100 m to almost 0.08 Sm^{-1} at 400 m. This is followed by a further small increase to 0.40 Sm^{-1} at 460–600 m, followed by a gentle decrease to 0.30 Sm^{-1} from 620–980 m. The location with the greatest increase in salinity from 500–600 m corresponds to one of the zones of higher transmissivity revealed by the differential flow log.

Hydrochemical logging: Measurements were carried out on 2005-07-12, i.e. about 14 days prior to the differential flow measurements. This showed a lower range of electrical conductivity values from 100–490 m (~ 0.05 Sm^{-1}), before increasing steadily to a maximum of 0.165 Sm^{-1} at 600 m and then decreasing to 0.135 Sm^{-1} at 940 m. Compared to the differential flow log data obtained later, there is little change in salinity from 100–400 m. From this level to the bottom of the borehole the flow log shows higher salinity, indicating a source of salinity that has entered the borehole, possibly from the high transmissive rock between 400–500 m.

The amount of drilling water in the borehole at the stage of the hydrochemical logging ranged from 0.58–1.73% from 40–440 m, followed by a rapid increase to 59% from 490 to 940 m. The total variation in chloride along the borehole is 12.2–399 mg/L Cl, i.e. fresh to brackish type groundwater mix.

Comment: The measured high transmissivities relate to the several deformation zones intercepted by KLX08 which, in turn, control the variation in salinity measured under natural and controlled conditions. Due to these zones much of the drilling water mixed with different groundwater sources (mostly from shallow to intermediate depths) have entered the rock mass from the borehole during drilling and subsequently under open hole conditions. Short circuiting therefore may be a major problem. The overall conclusion is that during open borehole conditions the groundwater that has preferentially infiltrated into the surrounding bedrock will first have to be removed with great care before 'representative' groundwater can be accessed.

References: SKB P-05-230, P-05-267, P-06-222, P-07-48, P-08-54.

C2.8.1 KLX08 (0–40.00 m; mid. vertical elevation: +7.02 m)

Cored Borehole					
Category	1	2	3	4	5
Drilling water (≤ 1%)				x	
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent				x	
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling				x	
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KLX08 between 2005-04-04 to 2005-06-13, i.e. sample collected in 2005-02-01 and used here. Na-HCO_3 type groundwater with low chloride (29.1 mg/L) and low drilling water content (0.24%), $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –75.0‰ VSMOW; tritium at 5.2 TU, $\delta^{13}C$ at –16.43‰ PDB and ^{14}C at 51.72 pmC.

Charge Balance: No measured Sicada value given but modelled PHREEQC value at +0.25%.

Time Series: Only one sample taken using tube sampling in 2005-07-12 (initial sample). Groundwater is fresh (16.3 mg/L Cl) with a drilling water content of 0.71%. Major ions incomplete, no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Lack of data.

Trace elements: Lack of data.

General: Na(Ca)-HCO_3 fresh groundwater, probably of recent recharge origin.

Comment: Despite the tube sample, and the absence of time series, incomplete major ions and lack of isotope data, the borehole section is reasonably constrained and the stability of the near-surface groundwater chemistry tends to be more predictable, therefore reflecting that expected at these shallow depths. Allocated Category 4.

C2.8.2 KLX08 (102.00–242.00 m; mid. vertical elevation: –124.54 m)

Cored Borehole **Category**	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)					x
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					x
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KLX08 between 2005-04-04 to 2005-06-13, i.e. sample collected in 2005-02-01 and used here. Na-HCO_3 type groundwater with low chloride (29.1 mg/L) and low drilling water content (0.24%), $\delta^{18}O$ at –10.9‰ VSMOW and δ^2H at –75.0‰ VSMOW; tritium at 5.2 TU, $\delta^{13}C$ at –16.43‰ PDB and ^{14}C at 51.72 pmC.

Charge Balance: Measured Sicada value given at –1.47%.

Time Series: Only one sample taken using the PLU hydraulic testing equipment in 2006-09-24. Groundwater is fresh (17.6 mg/L Cl) with a drilling water content of 0.22%. Major ions incomplete, Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Lack of data.

Trace elements: Lack of data.

General: Na(Ca)-HCO_3 fresh groundwater, probably of recent recharge origin.

Comment: Problem is the absence of time series, incomplete major ions and lack of trace and isotope data, and a 140 m long borehole section which may facilitate mixing/short circuiting. Allocated Category 5.

C2.8.3 KLX08 (241.00–341.00 m; mid. vertical elevation: –227.61 m)

Cored Borehole					
Category	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					x
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					x
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the L.2.3 dataset from the time of drilling borehole KLX08 between 2005-04-04 to 2005-06-13, i.e. sample collected in 2005-02-01 and used here. Na-HCO$_3$ type groundwater with low chloride (29.1 mg/L) and low drilling water content (0.24%), δ^{18}O at –10.9‰ VSMOW and δ^{2}H at –75.0‰ VSMOW; tritium at 5.2 TU, δ^{13}C at –16.43 PDB and ^{14}C at 51.72 pmC.

Charge Balance: Measured Sicada value given at –3.22%.

Time Series: Only one sample taken using the PLU hydraulic testing equipment in 2006-09-02. Groundwater is fresh (118 mg/L Cl) with a drilling water content of 2.66%. Major ions incomplete, no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Lack of data.

Trace elements: Lack of data.

General: Na-HCO$_3$(Cl) fresh groundwater, probably of recent recharge origin.

Comment: Problem is an absence of time series, incomplete major ions and lack of trace and isotope data, and a 100 m long borehole section which may facilitate mixing/short circuiting. Short circuiting/mixing is suggested from the amount of fresh groundwater at this depth. Allocated Category 5.

C2.8.4 KLX08 (357.00–497.00 m; mid. vertical elevation: –344.57 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					x
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					x
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KLX08 between 2005-04-04 to 2005-06-13, i.e. sample collected in 2005-02-01 and used here. Na-HCO_3 type groundwater with low chloride (29.1 mg/L) and low drilling water content (0.24%), $\delta^{18}O$ at –10.9‰ VSMOW and δ^2H at –75.0‰ VSMOW; tritium at 5.2 TU, ^{13}C at –16.43‰ PDB and ^{14}C at 51.72 pmC.

Charge Balance: Measured Sicada value given at –2.48%.

Time Series: Only one sample taken using the PLU hydraulic testing equipment in 2006-09-14. Groundwater is weakly brackish (270 mg/L Cl) with a drilling water content of 7.47%. Major ions incomplete, no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Lack of data.

Trace elements: Lack of data.

General: Na(Ca)-Cl(HCO_3,SO_4) weak brackish groundwater of mixed origin.

Comment: Problem is an absence of time series, > 5% drilling water, incomplete major ions and lack of trace and isotope data, and a 140 m long borehole section which may facilitate mixing/short circuiting. Short circuiting is suggested from the dilute nature of the groundwaters at this depth. Allocated Category 5.

C2.8.5 KLX08 (626.00–683.00 m; mid. vertical elevation: –539.39 m)

Cored Borehole					
Category	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					x
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					x
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					x
Major ions (incomplete)					
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KLX08 between 2005-04-04 to 2005-06-13, i.e. sample collected in 2005-02-01 and used here. Na-HCO$_3$ type groundwater with low chloride (29.1 mg/L) and low drilling water content (0.24%), δ^{18}O at –10.9‰ VSMOW and δ^{2}H at –75.0‰ VSMOW; tritium at 5.2 TU, δ^{13}C at –16.43 PDB and ^{14}C at 51.72 pmC.

Charge Balance: Measured Sicada value given at –0.44%.

Time Series: Only one sample taken using the PLU hydraulic testing equipment in 2007-08-15. Groundwater is brackish (2,200 mg/L Cl) with a drilling water content of 11.307%. Major ions complete.

Isotopes: Complete isotopes; no carbon isotopes (lack of HCO$_3$ ~ 25 mg/L). Tritium at 1.6 TU, and δ^{18}O at –14.8‰ VSMOW indicates a strong glacial component.

Trace elements: Good coverage.

General: Na(Ca)-Cl(SO$_4$) brackish glacial groundwater.

Comment: Problem is an absence of time series, > 10% drilling water, incomplete isotope data, and a 57 m long borehole section which may facilitate mixing/short circuiting. Short circuiting/mixing is suggested from the high drilling water content and measurable tritium component representing groundwaters from much shallower depths. On the other hand, brackish glacial groundwaters are common at this depth. Allocated Category 5.

C2.8.6 KLX08 (197.00–206.00 m; mid. vertical elevation: –150.43 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					x
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					x
Time series (inadequate)					
Time series absent					
Suitable section length					x
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					x
Major ions (incomplete)					
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KLX08 between 2005-04-04 to 2005-06-13, i.e. sample collected in 2005-02-01 and used here. Na-HCO_3 type groundwater with low chloride (29.1 mg/L) and low drilling water content (0.24%), $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –75.0‰ VSMOW; tritium at 5.2 TU, $\delta^{13}C$ at –16.43‰ PDB and ^{14}C at 51.72 pmC.

Charge Balance: Measured Sicada values given at –0.15% to +0.48%.

Time Series: 2005-12-01 to 2005-12-19 (18 days). Adequate time series (6 samples) showing a uniform salinity (12.40–12.80 mg/L Cl) supported by the remaining major ions. Drilling water content is consistently < 2% (1.29–1.55%) during the sampling period. Complete major ions.

Isotopes: Complete isotopes (3 samples); $\delta^{13}C$ at –17.58 to –17.55‰ PDB; ^{14}C at 62.69–63.00 pmC. Tritium at 1.4–2.9 TU and $\delta^{18}O$ at –10.7 to –10.4‰ VSMOW indicate a shallow recharge source.

Trace elements: Good coverage.

General: Na-HCO_3 fresh groundwater.

Comment: Problem is the presence of a shallow, fresh meteoric groundwater at –150.43 m elevation which shows little change in chemistry with time but indicates a steady increase in tritium content from 1.4–2.9 TU. Short circuiting/mixing is suspected, drawing groundwaters from shallower depths. Allocated Category 5.

C2.8.7 KLX08 (396.00–400.87 m; mid. vertical elevation: –320.03 m)

Cored Borehole					
Category	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					x
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					x
Time series (inadequate)					
Time series absent					
Suitable section length					x
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KLX08 between 2005-01-12 to 2005-06-13, i.e. sample collected in 2005-02-01 and used here. $Na\text{-}HCO_3$ type groundwater with low chloride (29.1 mg/L) and low drilling water content (0.24%), $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –75.0‰ VSMOW; tritium at 5.2 TU, $\delta^{13}C$ at –16.43‰ PDB and ^{14}C at 51.72 pmC.

Charge Balance: Measured Sicada values given at –1.28 to –0.15%.

Time Series: 2006-02-07 to 2006-03-06 (30 days). Adequate time series (8 samples) showing a uniform salinity (14.30–15.60 mg/L Cl) supported by the remaining major ions. Drilling water content is consistently < 2% (0.86–1.31%) during the sampling period. Complete major ions apart from TOC/DOC.

Isotopes: Complete isotopes (5 samples); $\delta^{13}C$ at –18.04 to –17.75% PDB; ^{14}C at 63.69–66.27 pmC. Tritium at 4.1–13.8 TU $\delta^{18}O$ at –10.8 to –10.7‰ VSMOW indicate a shallow recharge source.

Trace elements: Good coverage.

General: $Na\text{-}HCO_3$ fresh groundwater.

Comment: Problem is the presence of a shallow, meteoric fresh groundwater at –320.03 m elevation which shows little change in chemistry with time but indicates suspiciously high tritium contents. Short circuiting/mixing is suspected, drawing down fresh groundwaters from shallower depths. The high tritium is believed to be influenced by contamination (see section 3.1.1). Allocated Category 5.

C2.8.8 KLX08 (476.00–485.62 m; mid. vertical elevation: –390.71 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)		x			
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)		x			
Time series (inadequate)					
Time series absent					
Suitable section length		x			
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)		x			
Major ions (complete)		x			
Major ions (incomplete)					
Environmental isotopes (complete)		x*			
Environmental isotopes (incomplete)		x			
Monitoring borehole section					
Hydraulic effects (short circuiting)					

x* = One complete sample.

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KLX08 between 2005-04-04 to 2005-06-13, i.e. sample collected in 2005-02-01 and used here. Na-HCO_3 type groundwater with low chloride (29.1 mg/L) and low drilling water content (0.24%), $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –75.0‰ VSMOW; tritium at 5.2 TU, $\delta^{13}C$ at –16.43‰ PDB and ^{14}C at 51.72 pmC.

Charge Balance: Measured Sicada values given at –1.20% to +1.55% (the final sample 11160 at –11.88% is not considered due to > ±5%).

Time Series: On two occasions, from 2006-01-10 to 2006-01-12 (2 days) and from 2006-05-22 to 2006-06-26 (35 days). Adequate time series (2 + 12 samples) show a brackish groundwater with slightly lower salinity for the first sampling occasion (1,000–1,110 mg/L Cl) compared to the second occasion some 4 months later (1,480–1,600 mg/L Cl); both suggest stability during the sampling period. This stability is also reflected by the remaining major ions. Drilling water content is high for the initial sampling occasion (20.2–20.8%) and lower for the second occasion (4.93–5.89%). Complete major ions.

Isotopes: Incomplete isotopes apart for sample 11094 showing $\delta^{13}C$ at –15.70‰ PDB; ^{14}C at 32.09 pmC. Tritium at 1.70–756.60 TU suggesting contamination, and $\delta^{18}O$ at –15.70 to –14.90‰ VSMOW indicate a substantial glacial component. In the first sampling occasion $\delta^{18}O$ values are slightly more enriched at –14.00 to –13.60‰ VSMOW, but still indicating a significant glacial component.

Trace elements: Good coverage.

General: Na (Ca)-Cl (SO_4) brackish glacial groundwater.

Comment: The presence of irregular and high tritium contents is believed to be due to leaking tritiated water contamination from the pumping system (see section 3.1.1). Short circuiting is not thought to be an important factor at this level and the presence of brackish glacial groundwater is not unexpected; the analytical data are therefore considered to be representative during the second sampling occasion. Allocated Category 2.

C2.8.9 KLX08 (609.00–618.51 m; mid. vertical elevation: –504.54 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)			x		
Drilling water (> 10%)					
Time series (adequate)			x		
Time series (inadequate)					
Time series absent					
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)			x		
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KLX08 between 2005-04-04 to 2005-06-13, i.e. sample collected in 2005-02-01 and used here. Na-HCO_3 type groundwater with low chloride (29.1 mg/L) and low drilling water content (0.24%), $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –75.0‰ VSMOW; tritium at 5.2 TU, $\delta^{13}C$ at –16.43‰ PDB and ^{14}C at 51.72 pmC.

Charge Balance: Measured Sicada values given at –1.02% to +1.50%.

Time Series: 2006-07-03 to 2006-07-26 (23 days). Adequate time series (8 samples) show a fairly brackish groundwater composition with only a small decrease in salinity with time (2,010–2,030 mg/L Cl); this is supported by equally small increases in K, HCO_3 and SO_4, and decreases in Ca and Mg. Drilling water content is consistent at around 10% during the sampling period (10.70–11.20%). Complete major ions for some samples which include the selected sample.

Isotopes: Complete isotopes; no carbon isotopes (lack of HCO_3 at < 10 mg/L). Tritium varies from below detection (< 0.8 TU) to 2.5 TU during the sampling period indicating also a suspected contamination problem, in this section (cf. preceding sample above). $\delta^{18}O$ at –15.40 to –15.20‰ VSMOW indicates a high glacial component which shows a small systematic enrichment during the sampling period.

Trace elements: Good coverage of the selected sample.

General: Na(Ca)-Cl(SO_4) brackish glacial groundwater.

Comment: The data show some irregularities during sampling The tritium increase indicates possible contamination. However, the presence of brackish glacial groundwater at this depth is not unexpected, and the analytical data are therefore considered to be quite representative. Allocated Category 3.

KLX08: Tube samples sampled every 50 m from 90.00–940.00 m (2005-07-12) are considered unrepresentative and allocated Category 5.

C2.9 Description of Borehole KLX09

Borehole KLX09 is 880.38 m long (vertical depth of 874.07 m), cased to 100.6 m, and inclined at –84.93° from the horizontal. The borehole was drilled from 2005-08-26 to 2005-10-15 using HLX20 as a flushing water source to gain geological information at depth in the northwest part of the Laxemar subarea, for example, investigate the E-W, NW-SE, moderately northward dipping local major deformation zones (including ZSMEW007A) in the local model volume that are not associated with surface lineaments. The dominating rock type encountered consists of the Avrö granite (76.6%) with subsidiary fine-grained diorite-gabbro (10.1%) and fine-grained dioritoid (9.7%).

6.2.9.1 KLX09 (70.00–770.00 m; mid. vertical elevation: –71.90 to –765.85 m)

Available data to be evaluated consist only of tube samples taken every 50 m. The amount of residual flushing water present when hydrochemical logging was carried out in 2005-12-15 was low throughout the entire borehole (below 3% in all samples except the deepest sampled section, 770–820 m, where the uranine content was about 12%).

References: SKB P-06-47, P-06-164, P-06-240, P-08-33, P-08-54.

KLX09: Tube samples sampled every 50 m from 70.00–770.00 m (2005-12-15) are considered unrepresentative and allocated Category 5.

C2.10 Description of Borehole KLX10

Borehole KLX10 is 1,001.20 m long (vertical depth of 994.06 m), cased to 100.60 m, and inclined at –85.18° from the horizontal. The borehole was drilled from 2005-06-18 to 2005-10-15 to gain geological information in the central part of the Laxemar subarea and to facilitate hydrogeological and hydrochemical investigations at depth. The dominating rock type encountered consists of the Avrö granite and is characterised by a series of deformation zones mainly concentrated at 100–270 m and 330–350 m with more individual zones at about 440 m and 700 m borehole length. The distribution of total fractures in the core is typically in the range of 0–40 fractures m^{-1} to a length of 460 m. Below 460 m the fracture frequency is significantly reduced; however, minor sections with elevated fracture frequencies do occur.

Differential Flow Log: Measurements carried out in borehole KLX10 from 2005-12-08 to 2005-12-22 reveal transmissivities ranging from below detection at 10^{-9} m^2s^{-1} to $10^{-5.2}$ m^2s^{-1}; the high values characterise most of the borehole to about 440 m borehole length where they can be correlated to a series of 7–8 deformation zones of varying importance. From 440 m to the bottom of the borehole at about 1,000 m, both the number of deformation zones and their respective transmissivities decrease to just over 10^{-3} m^2s^{-1} at 540–560 m and 700–710 m, and to $10^{-3.4}$ m^2s^{-1} at 840 m. Otherwise, all values are below detection.

Under 'natural conditions' (i.e. no pumping) the groundwater flow is dominantly from the borehole to the surrounding bedrock at 130–210 m, 260 m, 320–330 m, 540 m and 700 m, where flow rates of 10^2–10^4 mLh^{-1} are recorded. Interestingly, from 355–440 m the natural flow is from the borehole to the bedrock (10^2–$10^{3.2}$ mL h^{-1}) which is an important observation influencing open-hole conditions when mixed groundwater in the borehole can contaminate the formation groundwaters in the bedrock close to the borehole. With pumping, all groundwater flow is towards the borehole with flow rates of $10^{3.2}$–$10^{5.2}$ mL h^{-1}.

Hydraulic injection tests have been conducted with the purpose of describing the rock hydraulic parameters adjacent to the borehole (mainly transmissivity), and thereby derive the hydraulic conductivity. The transmissivity measurements are in general agreement with the differential flow log interpretations.

Electrical Conductivity log: The hydraulic complexity of the open borehole conditions is further supported by the electrical conductivity log. Under 'natural' open hole conditions (i.e. no pumping), a fairly uniform salinity (~ 0.09 Sm^{-1}) is indicated from 100–200 m, followed by a fairly sharp increase between 200–320 m to 0.5 Sm^{-1}. The salinity increases more gradually to a maximum of 0.9 Sm^{-1} at 440 m remaining relatively stable to about 700 m and then decreasing gradually with depth recording ~ 0.35 Sm^{-1} at 1,000 m borehole length. During the pumping stage the greatest increases in salinity occur from 100–320 m (~ 0.2–0.3 Sm^{-1}) and a spike at 840 m (~ 1.5 Sm^{-1}). Otherwise, from 320–740 m and 890–1,000 m there is little change although there is an indication of a decrease in salinity from 540–720 m.

Hydrochemical logging: No hydrochemical borehole logging of KLX10 has been carried out.

Comment: The measured high transmissivities relate to the several deformation zones intercepted by KLX10 which, in turn, control the variation in salinity measured under natural and controlled conditions. Due to these zones much of the drilling water mixed with different groundwater sources (mostly from shallow to intermediate depths) have entered the rock mass from the borehole during drilling and subsequently under open hole conditions. Short circuiting therefore may be a major problem. The overall conclusion is that during open borehole conditions the groundwater that has preferentially infiltrated into the surrounding more transmissive bedrock sections will first have to be removed with great care before 'representative' groundwater can be accessed.

References: SKB P-06-58, P-06-116, P-06-182.

C2.10.1 KLX10 (0–100.60 m; mid. vertical elevation: –31.78 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)				x	
Time series absent					
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment				x	
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Drilling Water: Percussion borehole; no drilling water used.

Charge Balance: Measured Sicada values given at –0.62% to +0.14%.

Time Series: Percussion drilled part of KLX10 sampled from 2005-06-03 to 2005-06-07 (4 days) prior to the core drilling. Inadequate time series (2 samples) show a fresh groundwater composition (< 10 mg/L Cl) which, together with the other major ions, varies little during the sampling period. No drilling water values because of percussion drilling. Incomplete major ions; no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Lack of data.

Trace elements: Lack of data.

General: Na-HCO_3 fresh meteoric groundwater.

Comment: Problem is an absence of time series, incomplete major ion data, and an absence of isotope data and trace elements. Also, a long borehole section (100.6 m) which may facilitate mixing/short circuiting. However, because the near-surface groundwater chemistry is more predictable, it is considered to reflect that expected at these shallow depths. Allocated Category 4.

C2.10.2 KLX10 (351.00–368.00 m; mid. vertical elevation: –338.43 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)				?	
Time series (adequate)				x	
Time series (inadequate)					
Time series absent					
Suitable section length				x	
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section				x	
Hydraulic effects (short circuiting)				x?	

Drilling Water: HLX27 (6.01–164.70 m). Used for the first 10 days of drilling. Near-surface dilute brackish groundwater with 1,010 mg/L Cl, 175 mg/L HCO_3, 92 mg/L SO_4 and 4.16 mg/L Br. No further chemical or isotopic data are available.

HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). Used for continuation of the drilling for a 4 month period. There is one documented drilling water sample in the Extended L.2.3 dataset from the time just before drilling borehole KLX10 between 2005-06-18 and 2005-10-15, i.e. sample collected in 2005-02-01 and used here. Na-HCO_3 type fresh groundwater with low chloride (29.1 mg/L) and low drilling water content (0.24%), $\delta^{18}O$ at –10.9‰ VSMOW and δ^2H at –75.0‰ VSMOW; tritium at 5.2 TU, $\delta^{13}C$ at –16.43‰ PDB and ^{14}C at 51.72 pmC.

Charge Balance: Measured Sicada values given at –3.19% to –1.91%.

Time Series: Monitoring borehole section with sampling limited to two occasions in 2006-10-25 and 2007-06-28; salinity increase during this period (1,700–1,990 mg/L Cl) reflected by some of the other major ions (859–962 mg/L Na, 221–272 mg/L Ca, 32.3–39.3 mg/L Mg) but also decreases for K (7.41–6.70 mg/L), HCO_3 (98.4–80.5 mg/L) and SO_4 (284–167 mg/L). Drilling water content is high and decreases from 35.2–24.1% between the two sampling periods. Incomplete major ions; for the first sampling occasion no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC, and for the second sampling occasion no TOC/DOC.

Isotopes: Incomplete isotopes; no carbon isotopes. Tritium at 2.0–2.6 TU and $\delta^{18}O$ at –10.6 to –10.5‰ VSMOW.

Trace elements: Lack of data.

General: Na(Ca)-Cl(SO_4,HCO_3) brackish groundwater of mixed origin.

Comment: The high drilling water content recorded during the second sampling period in 2007-06-28 is believed to be anthropogenic in origin, resulting from the use of uranine in hydraulic tracer tests carried out from 2006-11-09 to 2006-11-16. Nevertheless, this does not explain the high drilling water value of 35.2% sampled on the first occasion prior to the tracer tests, although contamination from nearby boreholes cannot be excluded. Additional problems include a lack of time series data, incomplete major ion data, an absence of some isotope data and trace elements, and the possibility that tritium may be influenced by contamination. Despite these drawbacks, a Category 4 is allocated for the second sample.

C2.10.3 KLX10 (689.00–710.00 m; mid. vertical elevation: –676.19 m)

Cored Borehole					
Category	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)				?	
Time series (adequate)					
Time series (inadequate)				x	
Time series absent					
Suitable section length				x	
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section				x	
Hydraulic effects (short circuiting)				x?	

Drilling Water: HLX27 (6.01–164.70 m). Used for the first 10 days of drilling. Near-surface dilute brackish groundwater with 1,010 mg/L Cl, 175 mg/L HCO_3, 92 mg/L SO_4 and 4.16 mg/L Br. No further chemical or isotopic data are available.

HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). Used for continuation of the drilling for a 4 month period. There is one documented drilling water sample in the Extended L.2.3 dataset from the time just before drilling borehole KLX10 between 2005-06-18 and 2005-10-15, i.e. sample collected in 2005-02-01 and used here. Na-HCO_3 type fresh groundwater with low chloride (29.1 mg/L) and low drilling water content (0.24%), $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –75.0‰ VSMOW; tritium at 5.2 TU, $\delta^{13}C$ at –16.43‰ PDB and ^{14}C at 51.72 pmC.

Charge Balance: Measured Sicada values given at –2.12 to –1.00%.

Time Series: Monitoring borehole section with sampling limited to two occasions in 2006-10-25 and 2007-07-12; salinity is quite stable during these occasions (3,160–3,100 mg/L Cl) as are the other major ions apart from HCO_3 which decreases from 114–43 mg/L. Drilling water content is high increasing from 11.80 to 18.60% between the two sampling periods. Incomplete major ions; both sampling occasions have no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC, and the second sampling also no Mn.

Isotopes: Incomplete isotopes; no carbon isotopes. Tritium at 1.4–1.7 TU and $\delta^{18}O$ values at –10.6 to –10.1‰ VSMOW.

Trace elements: Lack of data.

General: $Na(Ca)-Cl(SO_4)$ brackish groundwater of mixed origin.

Comment: The high drilling water content recorded during the second sampling period in 2007-07-12 is probably of anthropogenic origin, resulting from the use of uranine in hydraulic tracer tests in the shallower section described above (351–368 m) carried out from 2006-11-09 to 2006-11-16. Short circuiting during sampling at this present depth may explain this contamination. Additional problems include the lack of time series data, incomplete major ion data, and an absence of some isotope data and trace elements. Despite these drawbacks, a Category 4 is allocated for the second sample.

C2.11 Description of Borehole KLX11A

Borehole KLX11A is 992.29 m long (vertical depth of 938.14 m), cased to 100.06 m, and inclined at –76.76° from the horizontal. The borehole was drilled from 2005-11-24 to 2006-03-02 and forms the deepest of seven boreholes ('nest') drilled at different orientation for detailed structural and hydraulic modelling of the upper approximately 100 m of bedrock. The borehole was drilled to gain geological information of the central part of the Laxemar subarea and to facilitate hydrogeological and hydrochemical investigations at depth. The dominating rock type encountered consists of the quartz monzodiorite with narrow bands of fine-grained diorite-gabbro (with sporadic fine-grained granite) in the upper approximately 600 m borehole length and pegmatite bands in the lower part.

Red staining with medium intensity is primarily noted in two intervals characterised by an elevated fracture frequency, i.e. from 250–260 m and 490–510 m. An increased fracture frequency is furthermore noted from 580–590 m and 850–860 m.

Differential Flow Log: Measurements carried out in borehole KLX11A from 2006-10-26 to 2006-11-10 reveal transmissivities ranging from below detection at 10^{-9} m^2s^{-1} to 10^{-5} m^2s^{-1}; higher values up to around 10^{-7} m^2s^{-1} characterise most of the borehole down to about 600 m borehole length, with highest values (just below 10^{-5} m^2s^{-1}) at 120–170 m, 265–305 m, 520 m and 580 m. From 600 m to the bottom of the borehole values are at or just above detection. Under 'natural conditions' (i.e. no pumping) the groundwater flow is dominantly from the borehole to the surrounding bedrock mostly at 110–180 m, 260–310 m and 440–600 m with flow rates ranging from about $10^{1.4}$–$10^{4.6}$ mL h^{-1}. Only at the shallowest level measured (~ 110 m) is the flow towards the open borehole with an average flow rate of $10^{3.3}$ mL h^{-1}. With pumping, all groundwater flow is towards the borehole at flow rates of $10^{1.2}$–$10^{5.2}$ mL h^{-1}.

Hydraulic injection tests have been conducted with the purpose of describing the hydraulic properties of the fracture zones and the rock parameters between them (mainly transmissivity). This was done at different measurement scales of 100 m, 20 m and 5 m sections. The transmissivity measurements are in general agreement with the differential flow log interpretations. For example, transmissivity profiles show two distinct zones. The first zone between 100 m and 600 m shows generally a relatively high and medium transmissisivity (except some sections with a transmissivity below $3{\cdot}10^{-9}$ m^2s^{-1}). The average transmissivity in this zone is $2.9{\cdot}10^{-6}$ m^2s^{-1}. The second zone between 600 m and 980 m shows relatively low transmissivities with an average transmissivity of $2.5{\cdot}10^{-10}$ m^2s^{-1}.

Electrical Conductivity log: The hydraulic complexity of the open borehole conditions is further supported by the electrical conductivity log. Under 'natural' open hole conditions (i.e. no pumping), a fairly uniform salinity (~ 0.05–0.06 Sm^{-1}) is indicated from 100–600 m, followed by a sharp but small increase at about 600 m to about 0.12 Sm^{-1} which continues steadily to the borehole bottom. During the pumping stage there is an irregular salinity increase (0.08–0.25 Sm^{-1}) between 100–300 m which remains quite steady to 580 m. Here, there is a small increase to 0.35 Sm^{-1} at 600 m and then a steady decrease to a pre-pumping value of about 0.12 Sm^{-1} at 800 m. The salinity increase down to about 600 m, and especially from 300–600 m, reflects the borehole lengths which have intercepted fracture zones of high transmissivity, and indicates the penetration of shallower, less saline groundwater into and along these zones during drilling and subsequent open-hole conditions. Pumping during the electrical conductivity measurements has removed these waters and replaced them by more representative formation groundwaters of higher salinity.

Hydrochemical logging: of the borehole was carried out on 2006-06-08, about 4.5 months prior to the differential flow measurements. This showed a similar range of electrical conductivity values from about 50–500 m (~ 0.05–0.06 Sm^{-1}), before increasing steadily to a maximum of 0.15 Sm^{-1} at about 600–700 m and then decreasing gradually to 0.06 Sm^{-1} at 935–985 m. By comparing these values with the later electrical conductivity logging described above, indicates the salinity lack of change due to open-hole effects during the 4.5 month interval between the two loggings. The amount of drilling water in the borehole during hydrochemical logging ranged from 4.76–6.37% for the upper 500 m of borehole length, followed by an increased range of 8.30–15.5% from 585–985 m. The total variation in chloride along the borehole is 28.7–53.3 mg/L Cl from 35–485 m, 311–323 mg/L Cl from 585–685 m and then a decrease of 138–60.2 mg/L Cl from 785–985 m, i.e. fresh to brackish type groundwater mix.

Comment: The measured high transmissivities relate to the several deformation zones intercepted by KLX11A which, in turn, control the variation in salinity measured under natural and controlled conditions. Due to these zones much of the drilling water mixed with different groundwater sources (mostly from shallow to intermediate depths) have entered the rock mass from the borehole during drilling and subsequently under open hole conditions. Short circuiting therefore may be a major problem. The overall conclusion is that during open borehole conditions the groundwater that has preferentially infiltrated into the surrounding bedrock will first have to be removed with great care before ‘representative’ groundwater can be accessed.

References: SKB P-06-180, P-06-201, P-06-306, P-07-24.

C2.11.1 KLX11A (35.00–85.00 m; mid. vertical elevation: –30.92 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)				x	
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent				x	
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling				x	
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HLX28 (6.03–154.20 m borehole length; mid. vertical elevation: –52.67 m). There are three documented drilling water samples used during drilling in the Extended L.2.3 dataset and these show good stability. Sample used here was collected in 2005-04-12 and chosen over the other earlier and later samples because it included isotope values. Na-HCO_3 type fresh groundwater with low chloride (23.0 mg/L) and $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –76.5‰ VSMOW; tritium at 1 TU, $\delta^{13}C$ at –16.15‰ PDB and ^{14}C at 46.91 pmC.

Charge Balance: Measured Sicada value given at +1.06%.

Time Series: Only one sample taken using tube sampling in 2006-06-08 (initial sample). Groundwater is fresh (49.5 mg/L Cl) with a drilling water content of 6.37%. Major ions incomplete, no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Incomplete: no carbon isotopes. Tritium at 5.0 TU and $\delta^{18}O$ at –10.80‰ VSMOW, both indicating a shallow bedrock component.

Trace elements: Lack of data.

General: Na(Ca)-HCO_3 fresh groundwater of recent recharge origin.

Comment: Despite the tube sample, and the absence of time series, incomplete major ions and isotope data, and the drilling water content, the borehole section is reasonably constrained and the stability of the near-surface groundwater chemistry tends to be more predictable, therefore reflecting that expected at these shallow depths. Category 4 allocated.

C2.11.2 KLX11A (516.50–519.50 m; mid. vertical elevation: –465.97 m)

Cored Borehole					
Category	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					x
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					x
Time series absent					
Suitable section length					x
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					x
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					x
Major ions (incomplete)					
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					
Monitoring borehole section					x
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX28 (6.03–154.20 m borehole length; mid. vertical elevation: –52.67 m). There are three documented drilling water samples used during drilling in the Extended L.2.3 dataset and these show good stability. Sample used here was collected in 2005-04-12 and chosen over the other earlier and later samples because it included isotope values. Na-HCO_3 type fresh groundwater with low chloride (39.3 mg/L) and $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –76.5‰ VSMOW; tritium at 1 TU, $\delta^{13}C$ at –16.15‰ PDB and ^{14}C at 46.91 pmC.

Charge Balance: Measured Sicada values given at –0.42% to +0.08%.

Time Series: Monitoring borehole section with sampling limited to two occasions in 2007-04-11 and 2007-07-24; salinity decreased somewhat during this period (145–105 mg/L Cl) also reflected by the other major ions apart from HCO_3 which increases from 218–248 mg/L. Drilling water content decreases from 4.56 to 2.69% between the two sampling periods. Complete major ions for the second sampling occasion; first occasion incomplete lacking S^{2-} and TOC/DOC.

Isotopes: Complete isotopes for the second sampling occasion; $\delta^{13}C$ at –17.30‰ PDB; ^{14}C at 64.70 pmC. Tritium at 5.87 TU and $\delta^{18}O$ at –11.30‰ VSMOW, both indicating a shallow bedrock component.

Trace elements: Good coverage for second sampling occasion.

General: Na(Ca)-HCO_3(Cl) fresh groundwater.

Comment: Fresh groundwater of mainly shallow bedrock origin. However, the recorded high drilling water content during both sampling periods may be of anthropogenic origin, resulting from the use of uranine in hydraulic tracer tests in the same section carried out from 2007-04-03 to 2007-04-05 and from 2007-07-24 to 2007-07-31. Short circuiting during sampling at this depth may also have contributed to residual uranine from similar tracer tests carried out in both shallower and deeper sections (see below). An additional problem is a lack of time series data and potential tritium contamination. However, the main problem is the lack of a representative groundwater composition from the depth sampled, and this can be traced back to inadequate pumping to remove the accumulated near-surface waters which have penetrated the bedrock fracture zones during drilling and subsequent open-hole conditions. Allocated Category 5.

C2.11.3 KLX11A (579.00–584.00 m; mid. vertical elevation: –526.01 m)

Cored Borehole **Category**	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					?
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					x
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					x
Major ions (incomplete)					
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					
Monitoring borehole section					x
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX28 (6.03–154.20 m borehole length; mid. vertical elevation: –52.67 m). There are three documented drilling water samples used during drilling in the Extended L.2.3 dataset and these show good stability. Sample used here was collected in 2005-04-12 and chosen over the other earlier and later samples because it included isotope values. Na-HCO_3 type fresh groundwater with low chloride (39.3 mg/L) and $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –76.5‰ VSMOW; tritium at 1 TU, $\delta^{13}C$ at –16.15‰ PDB and ^{14}C at 46.91 pmC.

Charge Balance: Measured Sicada value given as –0.22%.

Time Series: Monitoring borehole section with sampling limited to one occasion in 2007-04-02; salinity is low at 35.1 mg/L Cl and the drilling water content is 1.34%. Complete major ions.

Isotopes: Complete isotopes; δ^{13}C at –17.30‰ PDB; ^{14}C at 65.70 pmC. Tritium at 5.90 TU and δ^{18}O at –10.80‰ VSMOW, both indicating a shallow bedrock component.

Trace elements: Good coverage.

General: Na(Ca)-HCO_3 fresh groundwater.

Comment: Fresh groundwater of mainly shallow bedrock origin. The recorded drilling water content may be of anthropogenic origin, resulting from the use of uranine in hydraulic tracer tests in the same section carried out from 2007-03-22 to 2007-03-26. Short circuiting during sampling at this depth may also have contributed residual uranine from similar tracer tests carried out in both shallower and deeper sections (see above and below). An additional problem is an absence of time series data and potential tritium contamination. However, the main problem is the lack of a representative groundwater composition from the depth sampled, which differs little from the previous section. In common with the previous section, this can be traced back to inadequate pumping to remove the accumulated near-surface waters which have penetrated the bedrock fracture zones during drilling and subsequent open-hole conditions. Allocated Category 5.

C2.11.4 KLX11A (598.00–599.00 m; mid. vertical elevation: –542.07 m)

Cored Borehole					
Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)				?	
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent				x	
Suitable section length				x	
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)				x	
Major ions (incomplete)					
Environmental isotopes (complete)				x	
Environmental isotopes (incomplete)					
Monitoring borehole section				x	
Hydraulic effects (short circuiting)				x?	

Drilling Water: HLX28 (6.03–154.20 m borehole length; mid. vertical elevation: –52.67 m). There are three documented drilling water samples used during drilling in the Extended L.2.3 dataset and these show good stability. Sample used here was collected in 2005-04-12 and chosen over the other earlier and later samples samples because it included isotope values. Na-HCO_3 type fresh groundwater with low chloride (39.3 mg/L) and d δ^{18}O at –10.9‰ VSMOW and δ^{2}H at –76.5‰ VSMOW; tritium at 1 TU, δ^{13}C at –16.15‰ PDB and ^{14}C at 46.91 pmC.

Charge Balance: Measured Sicada value given as –0.64%.

Time Series: Monitoring borehole section with sampling limited to one occasion in 2007-06-13; salinity is 1,040 mg/L Cl and the drilling water content is 6.35%. Complete major ions.

Isotopes: Complete isotopes; $\delta^{13}C$ at –19.80‰ PDB; ^{14}C at 49.60 pmC. Tritium below detection (–0.80 TU), and $\delta^{18}O$ at –14.20‰ VSMOW indicates a strong glacial component.

Trace elements: Good coverage.

General: Na(Ca)-Cl(SO_4) brackish glacial groundwater.

Comment: Brackish glacial groundwater of mainly intermediate bedrock origin. The recorded drilling water content may be of anthropogenic origin, resulting from the use of uranine in hydraulic tracer tests in the same section carried out from 2007-04-24 to 2007-05-02 and from 2007-06-26 to 2007-7-09. Short circuiting during sampling at this depth may also have contributed to the transport of residual uranine from similar tracer tests carried out in shallower sections (see above). An additional problem is an absence of time series data. For this level, however, the groundwater sampled is not unusual in composition, and typical of the brackish glacial groundwaters found elsewhere at intermediate depths. In addition, there is good coverage of major and trace ions and isotopes. A problem of concern is the absence of time series. Allocated Category 4.

KLX11A: Tube samples sampled every 50 m from 135.00–985.00 m (2006-06-08) are considered unrepresentative and allocated Category 5.

C2.12 Description of Borehole KLX12A

Borehole KLX12A is 602.29 m long (vertical depth of 579.13 m), cased to 100.57 m, and inclined at –75.30° from the horizontal. The borehole was drilled from 2005-11-10 to 2006-03-04 to gain geological information in the central part of the Laxemar subarea and to further facilitate hydrogeological and hydrochemical investigations at depth. The dominating rock type encountered to around 450 m consists of Ävrö granite (with some sporadic narrow zones of diorite/gabbro and fine-grained granite) followed by major diorite/gabbro to 530 m and finally quartz monzodiorite to the maximum depth drilled.

Differential Flow Log: Measurements carried out in borehole KLX12A from 2006-06-09 to 2009-06-12 reveal transmissivities ranging from below detection at 10^{-9} m^2s^{-1} to 10^{-5} m^2s^{-1}; higher values up to about 10^{-7} m^2s^{-1} characterise most of the borehole length at 195 m, 230–259 m, 405 m and 540 m. Higher values (about $10^{-6.6}$ m^2s^{-1}) are recorded at 110–120 m and highest values (up to 10^{-5} m^2s^{-1}) at 140 m. Under 'natural conditions' (i.e. no pumping) the groundwater flow is dominantly from the borehole to the surrounding bedrock mostly at 100–140 m, 180–200 m, 230–270 m and at 550–540 m with flow rates ranging from $10^{1.4}$–$10^{3.4}$ mL h^{-1}. At one shallow level (~ 140–150 m) the flow is towards the open borehole with a flow rate of about $10^{3.9}$ mL h^{-1}, and at one deeper level (540 m) where the flow rate is low (about $10^{2.5}$ mL h^{-1} With pumping, all groundwater flow is reversed towards the borehole at flow rates of $10^{1.2}$–$10^{5.2}$ mL h^{-1}, including additional groundwaters from about 300–560 m.

Hydraulic injection tests have been conducted with the purpose of describing the hydraulic properties of the fracture zones and the rock parameters between them (mainly transmissivity). This was done at different measurement scales of 100 m, 20 m and 5 m sections. The transmissivity measurements are in general agreement with the differential flow log interpretations. For example, the highest transmissivity was located within the 144–164 m interval, with relatively high transmissivity within the 104–144 m and 224–264 m intervals.

Electrical Conductivity log: The hydraulic complexity of the open borehole conditions is further supported by the electrical conductivity log. Under 'natural' open hole conditions (i.e. no pumping), a fairly uniform salinity (~ 0.1 Sm^{-1}) is indicated from 100–280 m, followed by a steady increase to about ~ 0.5 Sm^{-1} which continues to 540 m, finally increasing to ~ 0.8 Sm^{-1} at the maximum depth measured. During the pumping stage the salinity increases to an elevated value of ~ 0.15 Sm^{-1} from 100–140 m. At 140–150 m there is a sharp increase to ~ 0.7 Sm^{-1} which continues to 400 m where a decrease to ~ 0.6 Sm^{-1} occurs to 440 m. Following this, there is a gradual increase to ~ 1.0 Sm^{-1} at 540 m before similar pre-pumping values at maximum depths (~ 0.9 Sm^{-1}) are achieved. The salinity increase from 150–400 m, and to a lesser extent from 500.550 m, reflects the borehole lengths which are characterised by high to relatively high transmissivities, and indicates the penetration of shallower, less saline groundwater into and along these zones during drilling and subsequent open-hole conditions. Subsequent pumping during the electrical conductivity measurements has removed some or most these waters and replaced them by more representative formation groundwaters of higher salinity. This effect is much less marked at greater depth, where the overall transmissivity is lower.

Hydrochemical logging: This was carried out in the borehole on 2006-04-11, about two months prior to the differential flow measurements. The hydrochemical logging showed a similar pattern and range of electrical conductivity values to the differential flow log measurements with constant salinity to about 200 m followed by a gradual increase with increasing depth to the borehole bottom. Little change has occurred during the two month period between the respective measurements. The amount of drilling water in the borehole during hydrochemical logging ranged from 3.12–4.74% for the upper 300 m of borehole length, followed by a steady increase to 32.3% at 595 m. The total variation in chloride along the borehole is 179–2,960 mg/L, i.e. fresh to brackish type groundwater mix. A small depletion of $\delta^{18}O$ from –11.1 to –12.0 VSMOW is indicated.

Comment: The measured high transmissivities relate to the several fracture zones intercepted by KLX12A which, in turn, control the variation in salinity measured under natural and controlled conditions. Due to these zones much of the drilling water mixed with different groundwater sources (mostly from shallow to intermediate depths) have entered the rock mass from the borehole during drilling and subsequently under open hole conditions. Short circuiting therefore may be a major problem. The overall conclusion is that during open borehole conditions the groundwater that has preferentially infiltrated into the surrounding bedrock will first have to be removed with great care before 'representative' groundwater can be accessed.

References: SKB P-06-142, P-06-148, P-06-185, P-06-259, P-06-305.

C2.12.1 KLX12A (35.00–85.00 m; mid. vertical elevation: –30.92 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)				x	
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent				x	
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling				x	
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset close to the time of drilling borehole KLX12A between 2005-11-10 to 2006-03-04, i.e. sample collected in 2005-10-28 and used here. Na-HCO_3 type groundwater with low chloride (31.9 mg/L), $\delta^{18}O$ at –10.8‰ VSMOW and $\delta^{2}H$ at –76.9‰ VSMOW; tritium at 5.7 TU, $\delta^{13}C$ at –16.12‰ PDB and ^{14}C at 52.73 pmC.

Charge Balance: Measured Sicada value given at +1.06%.

Time Series: Only one sample taken using tube sampling in 2006-06-08 (initial sample). Groundwater is fresh (182 mg/L Cl) with a drilling water content of 6.37%. Major ions incomplete, no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Incomplete: no carbon isotopes no tritium. $\delta^{18}O$ at –11.10‰ VSMOW.

Trace elements: Lack of data.

General: Na(Ca)-HCO_3(Cl) fresh groundwater probably of recent recharge origin.

Comment: Despite the tube sample, and the absence of time series, incomplete major ions and isotope data, and the drilling water content, the borehole section is reasonably constrained and the stability of the near-surface groundwater chemistry tends to be more predictable, therefore reflecting that expected at these shallow depths. Allocated Category 4.

C2.12.2 KLX12A (535.00–545.00 m; mid. vertical elevation: –501.12 m)

Cored Borehole					
Category	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)				x	
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)				x	
Time series absent					
Suitable section length				x	
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)				x	
Environmental isotopes (incomplete)					
Monitoring borehole section				x	
Hydraulic effects (short circuiting)					

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset close to the time of drilling borehole KLX12A between 2005-11-10 to 2006-03-04, i.e. sample collected in 2005-10-28 and used here. Na-HCO_3 type groundwater with low chloride (31.9 mg/L), $\delta^{18}O$ at –10.8‰ VSMOW and $\delta^{2}H$ at –76.9‰ VSMOW; tritium at 5.7 TU, $\delta^{13}C$ at –16.12‰ PDB and ^{14}C at 52.73 pmC.

Charge Balance: Measured Sicada values given at –1.23 to –0.92%.

Time Series: Monitoring borehole section with sampling limited to two occasions in 2006-11-14 and 2007-07-11; salinity has increased during this period (2,220–3,080 mg/L Cl) as do the other major ions apart from HCO_3 which decreases from 91.8–47.10 mg/L. Drilling water content decreases from 7.10 to 5.71% between the two sampling periods. Complete major ions for the first sampling occasion; second occasion incomplete lacking S^{2-}.

Isotopes: Complete isotopes for the second sampling occasion; $\delta^{13}C$ at –22.60‰ PDB; ^{14}C at 57.00 pmC. Tritium at 1.90 TU and $\delta^{18}O$ at –12.30‰ VSMOW, both indicating an intermediate bedrock composition with a possible weak glacial component. In comparison, the first sampling shows a higher tritium content (2.5 TU) and a more enriched $\delta^{18}O$ value at –11.70‰ VSMOW.

Trace elements: Good coverage on both sampling occasions.

General: Na(Ca)-Cl(SO_4) brackish groundwater.

Comment: Brackish groundwater of mainly intermediate bedrock origin. The recorded drilling water content during both sampling periods is not considered to be of anthropogenic origin as no hydraulic tracer tests were carried out in this borehole, or boreholes in the near vicinity. An additional problem is a lack of time series data and possible tritium contamination. However, comparing the two sampling periods indicates that the second sample with a decrease in drilling water, increasing mineralisation and a more depleted $\delta^{18}O$ value, is approaching a composition more expected for the depth sampled, namely a brackish glacial groundwater. Category 4 allocated for the second sample.

KLX12A: Tube samples sampled every 50 m from 145.00–595.00 m (2006-04-11) are considered unrepresentative and allocated Category 5.

C2.13 Description of Borehole KLX13A

Borehole KLX13A (designated chemistry borehole) is 595.85 m long (vertical depth of 591.22 m), cased to 99.96 m, and inclined at –82.23° from the horizontal. The borehole was drilled from 2006-05-19 to 2006-08-16 to gain geological information of the northwest part of the Laxemar subarea and to facilitate further investigations in hydrogeology and hydrochemistry at depth. The dominating rock type encountered throughout the borehole consists of Ävrö granite with sporadic zones of varying thickness (to a maximum of about 40 m) of diorite/gabbro and in one case fine-grained diorite-gabbro. A series of six minor deformation zones characterise the borehole down to about 400 m and a major deformation zone from about 500 m to the borehole bottom at 596 m.

Differential Flow Log: Measurements carried out in borehole KLX13A from 2006-09-21 to 2006-10-01 reveal transmissivities ranging from below detection at 10^{-9} m^2s^{-1} to 10^{-5} m^2s^{-1}; higher values up to and just under about 10^{-6} m^2s^{-1} characterise most of the borehole length from 320–500 m, and up to and just under 10^{-7} m^2s^{-1} from 157–230 m and 540–560 m. The highest values occur at about 120 m ($10^{-5.9}$ m^2s^{-1}) and 390 m ($10^{-5.2}$ m^2s^{-1}). Lower transmissivity values (~ 10^{-9}–10^{-8} m^2s^{-1}) occur from 230–300 m and from 570–590 m. Under 'natural conditions' (i.e. no pumping) there is a clear subdivision between natural flow from the bedrock to the borehole from 100–240 m with flow rates mostly of 10^1–10^3 mL h^{-1}, and from the borehole out into the surrounding bedrock from 290–560 m with flow rates of 10^2–10^4 mL h^{-1}. With pumping, all groundwater flow is reversed towards the borehole at flow rates from $10^{1.2}$–$10^{6.1}$ mL h^{-1}, including additional groundwaters particularly from about 240–280 m and about 580 m with flow rates of 10^2–10^3 mL h^{-1}.

Hydraulic injection tests have been conducted with the purpose of describing the hydraulic properties of the fracture zones and the rock parameters between them (mainly transmissivity). This was done at different measurement scales of 100 m and 20 m sections. The transmissivity measurements are in general agreement with the differential flow log interpretations.

Electrical Conductivity log: The hydraulic complexity of the open borehole conditions is further supported by the electrical conductivity log. Under 'natural' open hole conditions (i.e. no pumping), a fairly uniform salinity (~ 0.04 Sm^{-1}) is indicated from 100–560 m, followed by a sharp increase to about 0.2 Sm^{-1} which continues to 590 m. During the pumping stage the salinity increases but remains uniform from 100–395 m at an elevated salinity of just over ~ 0.1 Sm^{-1}. Following a small sharp increase to 0.2 Sm^{-1}, the salinity increases irregularly to 0.4 Sm^{-1} from 395–560 m before decreasing to 0.02 Sm^{-1} at the end of the borehole. The salinity increase along the full length of the borehole reflects the overall high transmissivities of the bedrock and indicates the penetration of shallower, less saline groundwater into and along the bedrock during drilling and subsequent open-hole conditions. Subsequent pumping during the electrical conductivity measurements has removed a percentage of these waters and replaced them by more representative formation groundwaters of higher salinity.

Hydrochemical logging: of the borehole was carried out on 2006-09-19, about two days prior to the differential flow measurements. The hydrochemical logging showed a similar pattern and range of electrical conductivity values with constant salinity to about 500 m followed by a sharp increase to the end of the borehole. Little change has occurred during the two day period between the respective measurements. The amount of drilling water in the borehole during hydrochemical logging was very low, ranging from 0.07–0.18% to about 500 m depth followed by a rapid increase to 41.8% at the end of the borehole at 585 m. The total variation in chloride along the borehole is 19.3–29.8 mg/L to 500 m depth followed by an increase to 502 mg/L at the end of the borehole, i.e. transition from a fresh to a brackish type groundwater mix.

Comment: The measured high transmissivities relate to the several deformation zones intercepted by KLX13A which, in turn, control the variation in salinity measured under natural and controlled conditions. During drilling of the borehole up to 782 m^3 of flushing were consumed and the volume of returned water pumped from the borehole by air-lift pumping during drilling was 4,001 m^3. The uranine budget suggests that no flushing water has been lost to the borehole and to the adjacent host bedrock during drilling, which is difficult to explain considering the amount of drilling water that has been recorded during sampling (see below). Due to the high transmissive deformation zones, much of this drilling water mixed with different groundwater sources (mostly from shallow to intermediate depths) have entered the rock mass from the borehole during drilling and subsequently under open hole conditions. These waters will first have to be removed with great care before 'representative' groundwater can be accessed. Short circuiting therefore may be a major problem.

References: SKB P-06-245, P-06-280, P-07-99, P-07-149, P-07-195.

C2.13.1 KLX13A (35.00–85.00 m; mid. vertical elevation: –35.34 m)

Cored Borehole					
Category	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)				?	
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent				x	
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling				x	
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Drilling Water: HLX14 (11.90–115.90 m; mid. vertical elevation: –42.17 m). There is one documented drilling water sample in the Extended L.2.3 dataset close to the time of drilling borehole KLX13A between 2006-05-19 to 2006-08-16, i.e. sample collected in 2006-11-04 and used here. Na-Cl,HCO$_3$(SO$_4$) brackish mix type groundwater with chloride at 357 mg/L, bicarbonate at 223 mg/L, sulphate at 56.3 mg/L, δ^{18}O at –11.12‰ VSMOW and δ^{2}H at –84.4‰ VSMOW; tritium at 2.5 TU, δ^{13}C at –17.20 PDB and ^{14}C at 49.70‰ pmC.

Charge Balance: Measured Sicada value given at +1.82%.

Time Series: Only one sample taken using tube sampling in 2006-09-19 (initial sample). Groundwater is fresh (29.8 mg/L Cl) with a drilling water content of 0.18% (probably contamination). Major ions incomplete, no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Lack of data.

Trace elements: Lack of data.

General: $Ca(Na)\text{-}HCO_3$ fresh groundwater.

Comment: Despite the tube sample, and the absence of time series, incomplete major ions and no isotope or trace element data, the borehole section is reasonably constrained and the stability of the near-surface groundwater chemistry tends to be more predictable, therefore reflecting that expected at these shallow depths. Allocated Category 4.

C2.13.2 KLX13A (486.85–595.85 m; mid. vertical elevation: –512.97 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					x
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					x
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX14 (11.90–115.90 m; mid. vertical elevation: –42.17 m). There is one documented drilling water sample in the Extended L.2.3 dataset close to the time of drilling borehole KLX13A between 2006-05-19 to 2006-08-16, i.e. sample collected in 2006-11-04 and used here. $Na\text{-}Cl,HCO_3(SO_4)$ brackish mix type groundwater with chloride at 357 mg/L, bicarbonate at 223 mg/L, sulphate at 56.3 mg/L, $\delta^{18}O$ at –11.12‰ VSMOW and $\delta^{2}H$ at –84.4‰ VSMOW; tritium at 2.5 TU, $\delta^{13}C$ at –17.20 PDB and ^{14}C at 49.70‰ pmC.

Charge Balance: Measured Sicada value given at –0.31%.

Time Series: Only one sample taken using the PLU hydraulic testing equipment in 2006-08-25. Groundwater is brackish (1,070 mg/L Cl) with a drilling water content of 16.90%. Major ions incomplete, no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Complete isotopes; $\delta^{13}C$ at –18.30‰ PDB; ^{14}C at 44.40 pmC. Tritium under detection (–0.80 TU), and $\delta^{18}O$ at –15.40‰ VSMOW indicating a strong glacial component.

Trace elements: Lack of data.

General: $Na(Ca)\text{-}Cl(HCO_3,SO_4)$ brackish glacial groundwater of mixed origin.

Comment: Problem is an absence of time series, incomplete major ions and lack of trace element data, high drilling water content, and a 109 m long borehole section which may facilitate mixing/short circuiting. Allocated Category 5.

C2.13.3 KLX13A (432.00–439.16 m; mid. vertical elevation: –408.01 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)			x		
Drilling water (> 10%)					
Time series (adequate)			x		
Time series (inadequate)					
Time series absent					
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)			x		
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)			x?		

Drilling Water: HLX14 (11.90–115.90 m; mid. vertical elevation: –42.17 m). There is one documented drilling water sample in the Extended L.2.3 dataset close to the time of drilling borehole KLX13A between 2006-05-19 to 2006-08-16, i.e. sample collected in 2006-11-04 and used here. Na-Cl,HCO_3(SO_4) brackish mix type groundwater with chloride at 357 mg/L, bicarbonate at 223 mg/L, sulphate at 56.3 mg/L, δ^{18}O at –11.12‰ VSMOW and δ^{2}H at –84.4‰ VSMOW; tritium at 2.5 TU, δ^{13}C at –17.20 PDB and ^{14}C at 49.70‰ pmC.

Charge Balance: Measured Sicada values given at –1.68 to 3.02%.

Time Series: 2006-12-18 to 2007-01-21 (34 days). Adequate time series (7 samples) show a fairly brackish, relatively stable groundwater composition with only a small systematic decrease in salinity with time (762–733 mg/L Cl); this is accompanied by equally small decreases in K and Ca, and increases in HCO_3. Drilling water content decreases from 11.40 to 8.75% during the sampling period. Complete major ions.

Isotopes: Complete isotopes; δ^{13}C variable at –17.11 to –13.70‰ PDB; ^{14}C variable at 21.71–47.41 pmC. Tritium varies from below detection (< 0.8 TU) to 11.5 TU during the sampling period, and δ^{18}O values at –15.90 to –15.70‰ VSMOW indicate a high glacial component.

Trace elements: Good coverage.

General: Na(Ca)-Cl(HCO_3) brackish glacial groundwater.

Comment: Although there are adequate time series data and the major ions are reasonably stable, there is some systematic change in the composition with time. This seems to have influenced the ^{14}C isotope data which are unstable. There are also a marked changes in tritium which are considered to indicate contamination, i.e. large variation in tritium (values up to 11.5 TU) without any correlation with δ^{18}O. Nevertheless, a sample has been chosen to best represent the groundwaters at this depth, based on comparison with the shallower section described above (and other boreholes) sampled at an earlier stage. Allocated Category 3.

C2.13.4 KLX13A (499.50–506.66 m; mid. vertical elevation: –474.99 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)				?	
Time series (adequate)					
Time series (inadequate)				x	
Time series absent					
Suitable section length				x	
Sampling during sampling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Drilling Water: HLX14 (11.90–115.90 m; mid. vertical elevation: –42.17 m). There is one documented drilling water sample in the Extended L.2.3 dataset close to the time of drilling borehole KLX13A between 2006-05-19 to 2006-08-16, i.e. sample collected in 2006-11-04 and used here. Na-Cl,HCO_3(SO_4) brackish mix type groundwater with chloride at 357 mg/L, bicarbonate at 223 mg/L, sulphate at 56.3 mg/L, $\delta^{18}O$ at –11.12‰ VSMOW and $\delta^{2}H$ at –84.4‰ VSMOW; tritium at 2.5 TU, $\delta^{13}C$ at –17.20 PDB and ^{14}C at 49.70‰ pmC.

Charge Balance: Measured Sicada values given at –1.55 to –0.07%.

Time Series: 2006-11-23 to 2006-12-11 (18 days). Reasonable time series (4 samples) show a fairly brackish, stable groundwater composition (ranging from 678–774 mg/L) with no obvious trend during sampling; however, small systematic decreases in Na, K, Ca and Mg are recorded. Drilling water content is variable from 14.10 to 16.60% during the sampling period. Incomplete major ions; no TOC.

Isotopes: Incomplete isotopes; no carbon isotopes. Tritium varies between 0.9–10.20 TU and contamination is suspected; $\delta^{18}O$ at –15.20 to –14.60‰ VSMOW indicates a high glacial component.

Trace elements: Lack of data.

General: Na(Ca)-Cl(HCO_3) brackish glacial groundwater.

Comment: Although reasonable time series data, there is some indication of systematic change during the sampling period which may reflect short circuiting (e.g. increased depletion of ^{18}O). Furthermore, there is high drilling water content, inadequate isotope data, no trace element data and the tritium contents are suspect probably due to contamination and some short circuiting. Nevertheless, such brackish glacial groundwater is considered typical for such depths, and the sample chosen for Category 4 is that taken at an early stage in the sampling recording the lowest tritium content (0.9 TU) and thus maybe considered the most suitable.

KLX13A: Tube samples sampled every 50 m from 135.00–485.00 m (2006-09-19) are considered unrepresentative and allocated Category 5.

C2.14 Description of Borehole KLX15A

Borehole KLX15A (designated chemistry borehole) is 1,000.43 m long (vertical depth of 754.58 m), cased to 76.13 m, and inclined at –54.41° from the horizontal. The borehole was drilled from 2007-01-17 to 2007-02-25 with the objective of: a) investigating the geometry of the quartz monzodiorite in the southern part of the candidate site, b) locating the position of modelled deformation zone ZSMNW042A, and 3) characterising groundwater from repository depths characterised by the quartz monzodiorite. The dominant rock type encountered throughout the borehole consists of quartz monzodiorite with sporadic thin zones of, in decreasing frequency, fine-grained granite, Ävrö granite and fine-grained diorite-gabbro. Fairly evenly distributed along the borehole are 20 deformation zones of varying importance.

Differential Flow Log: Measurements carried out in borehole KLX15A from 2007-05-02 to 2007-05-18 reveal transmissivities ranging from below detection at 10^{-9} m^2s^{-1} to 10^{-5} m^2s^{-1}; higher values up to and just under about 10^{-6} m^2s^{-1} characterise most of the borehole length from 80–200 m, 380–410 m and 630–640 m. The highest values occur at about 130–140 m (10^{-5} m^2s^{-1}) and about 260 m ($10^{-5.7}$ m^2s^{-1}). Lower transmissivity values (~ 10^{-9}–10^{-7} m^2s^{-1}) occur at about 450–460 m, about 500 m and 840–850 m. Transmissivities at or below detection characterise most of the bedrock between 200–370 m and from 440 to the end of the borehole. Under 'natural conditions' (i.e. no pumping) only at 100–160 m and at about 500 m is the water flow from the borehole out into the host bedrock at flow rates ranging from 10^2–10^4 mL h^{-1}. At about 200 m, 260 m, 390–410 m and at 630–640 m, the flow is into the borehole from the bedrock with flow rates mostly ranging from 10^2–10^4 mL h^{-1}, and from borehole out into the surrounding bedrock from 290–560 m with flow rates of 10^2–10^4 mL h^{-1}. With pumping, all groundwater flow is towards the borehole with major flow rates of $10^{1.3}$–$10^{4.2}$ mL h^{-1} at 80–200 m and at 260–270 m, and of $10^{2.5}$–$10^{5.3}$ mL h^{-1} at 370–410 m.

No hydraulic injection tests have been conducted in borehole KLX15A.

Electrical Conductivity log: The hydraulic complexity of the open borehole conditions is further supported by the electrical conductivity log. Under 'natural' open hole conditions (i.e. no pumping), the salinity at 120 m (~ 0.05 Sm^{-1}) increases sharply to 0.45–0.50 Sm^{-1} and this remains uniform to 390 m. Here, there is a gradual increase to 1.0 Sm^{-1} from 390 to 540 m, and this salinity continues close to the bottom of the borehole at 960 m, whereupon there is a small increase to about 2.0 Sm^{-1} down to 980 m. During the pumping stage, the salinity along the borehole increases with a sharp increase to 0.4 Sm^{-1} at 140 m followed by a sharp increase to 0.9 Sm^{-1} at the same depth, and remains at this value to 390 m. Here there is a small increase to 1.8 Sm^{-1} which continues to 640 m and then decreasing a little down to 940 m at 1.5 Sm^{-1}. This is followed by a small increase to 2 Sm^{-1} down to 980 m.

The salinity increase with pumping is greatest down to 140 m and this corresponds to the high transmissivity of the bedrock at this depth; the remainder of the borehole is less transmissive and correspondingly the salinity increase with pumping is less marked as there are less contaminated waters to be removed.

Drilling consumed 1,057 m^3 of flushing water and the volume of returned water pumped from the borehole by air-lift pumping during drilling was 1,710 m^3. The uranine budget suggests that flushing water has been lost to the borehole and the adjacent host bedrock during drilling. This is supported by the presence of flushing water (4–14%) in the samples collected from section 623.0–634.5 m (see below).

Hydrochemical logging: No hydrochemical logging was carried out in KLX15A.

Comment: The measured high transmissivities relate to one or more deformation zones intercepted by KLX15A which, in turn, control the variation in salinity measured under natural and controlled conditions. Due to these high transmissive zones much of the drilling water mixed with different groundwater sources (mostly from shallow to intermediate depths) have entered the rock mass from the borehole during drilling and subsequently under open hole conditions. Short circuiting therefore may be a major problem. The overall conclusion is that during open borehole conditions the groundwater/flushing water mixtures that are present in the surrounding bedrock will first have to be removed with great care before 'representative' groundwater can be accessed.

References: SKB P-07-176, P-08-58, P-08-69.

C2.14.1 KLX15A (623.00–634.51 m; mid. vertical elevation: –467.22 m)

Cored Borehole					
Category	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)					
Drilling water (≤ 5%)		x			
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)		x			
Time series (inadequate)					
Time series absent					
Suitable section length		x			
Sampling during sampling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)		x			
Major ions (complete)		x			
Major ions (incomplete)					
Environmental isotopes (complete)		x			
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HLX14 (11.90–115.90 m; mid. vertical elevation: –42.17 m). There are no documented drilling water samples in the Extended L.2.3 dataset during drilling of borehole KLX15A between 2007-01-17 to 2007-02-25. The closest data are from 2006-11-04, and this is used here. Na-HCO_3(Cl) brackish groundwater with low chloride (357 mg/L) and low drilling water content (0.5%) with $\delta^{18}O$ at –11.2‰ VSMOW and $\delta^{2}H$ at –84.4‰ VSMOW; tritium at 2.5 TU, $\delta^{13}C$ at –17.20‰ PDB and ^{14}C at 49.7 pmC.

Charge Balance: Measured Sicada values given at –2.55 to +0.01% (sample 11929 was omitted because of charge balance > 5%).

Time Series: 2007-06-28 to 2007-08-06 (39 days). Adequate time series (9 samples) show a brackish groundwater composition with a small systematic increase in salinity with time (5,670–5,890 mg/L Cl); this is accompanied by equally small increases in Ca and Mg, and decreases in K and HCO_3. Drilling water content decreases from 7.55 to 4.43% during the sampling period. Complete major ions.

Isotopes: Complete isotopes; no carbon isotopes (inadequate HCO_3; < 20 mg/L). Tritium varies from below detection (< 0.8 TU) to 1.39 TU during the sampling period and $\delta^{18}O$ at –10.90 to –10.70‰ VSMOW.

Trace elements: Good coverage.

General: Na(Ca)-Cl(SO_4) brackish groundwater with a possible weak marine component (52–56 mg/L Mg).

Comment: Although there is adequate time series data and the major ions are reasonably stable, there is an indication of a systematic change during the sampling period which may correlate with a decrease in the drilling water component. Because of the presence of > 1% drilling water and the instability for some ions during the sampling period, a Category 2 has been allocated.

C2.15 Description of Borehole KLX16A

No borehole description is given as only tube sampling was carried out at one level.

6.2.15.1 KLX16A (60.99–410.00 m; mid. vertical elevation: –58.09 to –327.97 m)

KLX16A: Tube samples sampled every 50 m from 60.00–410.00 m (2007-02-06) are considered unrepresentative and allocated Category 5. No other chemical data are available for this borehole.

C2.16 Description of Borehole KLX17A

Borehole KLX17A (designated chemistry borehole) is 701.08 m long (vertical depth of 600.10 m), cased to 65.42 m, and inclined at –61.33° from the horizontal. The borehole was drilled from 2006-09-13 to 2006-10-23 with the objective of locating the position of deformation zones ZSMEW900B and ZSMEW900A,and characterising the hydrogeology and hydrochemistry from repository depths in the north-west of the candidate area characterised by Ävrö granite. The dominating rock type encountered throughout the borehole consists of Ävrö granite with sporadic intercalations of varying thickness (to a maximum of less than 10 m) of diorite/gabbro, fine-grained diorite-gabbro and fine-grained granite. From 485 m to the maximum depth drilled, the borehole is free from intercalations apart from one minor fine-grained granite zone at about 575 m. A series of ten deformation zones characterise the borehole with two major deformation zones at about 105–120 m and 190–230 m borehole length.

Differential Flow Log: Measurements carried out in borehole KLX17A from 2006-12-07 to 2007-01-09 reveal transmissivities ranging from below detection at 10^{-9} m^2s^{-1} to 10^{-5} m^2s^{-1}; higher values between about 10^{-6}–10^{-7} m^2s^{-1} characterise the borehole length from 80–110 m, 180–200 m and about 315 m. The highest values at or just above 10^{-5} m^2s^{-1}occur at 110 m and about 420–430 m. Lower transmissivity values (~ 10^{-9}–10^{-8} m^2s^{-1}) occur at about 245 m, 290 m, 320–340 m, 370 m, 410 m and 470 m. Under ‘natural conditions’ (i.e. no pumping) there is a clear subdivision between natural flow from the bedrock to the borehole from about 85–110 m and 185–200 m with flow rates ranging from $10^{2.1}$–$10^{4.1}$ mL h^{-1}, and from the borehole out into the surrounding bedrock at about 320 m and from 420–430 m with flow rates of about $10^{2.4}$ and $10^{4.1}$ mL h^{-1} respectively. With pumping, all groundwater flow is reversed towards the borehole, including additional groundwaters particularly from about 210–430 m, 465 m and 665–680 m with flow rates ranging from about $10^{0.5}$–$10^{5.2}$ mL h^{-1}.

Hydraulic injection tests have been conducted with the purpose of describing the hydraulic properties of the fracture zones and the rock parameters between them (mainly transmissivity). This was done at different measurement scales of 100 m, 20 m and 5 m sections. The transmissivity measurements are in general agreement with the differential flow log interpretations. Of interest is the possibility of larger transmissive zones in the borehole vicinity which could be attributed to steep fractures that do not intersect the borehole, but are connected by lower transmissive fractures. Short circuiting, therefore, may be a problem during groundwater sampling.

Electrical Conductivity log: The hydraulic complexity of the open borehole conditions is further supported by the electrical conductivity log. Under ‘natural’ open hole conditions (i.e. no pumping), a fairly uniform salinity (~ 0.04–0.05 Sm^{-1}) is indicated from 80–440 m, followed by a sharp increase to about ~ 0.1 Sm^{-1} which continues to the end of the borehole at about 700 m. During the pumping stage the salinity to increases to an elevated value of about 0.1.5 Sm^{-1} from about 80–110 m. Following a small sharp increase to just over 0.2 Sm^{-1} at 105 m, the salinity remains between 0.2–0.3 Sm^{-1} to about 420 m whereupon there is a small systematic decrease to 0.2 Sm^{-1} at about 580 m which continues to about 680 m. The final 20 m of the borehole suggests a rise in salinity to 0.3 Sm^{-1}. The salinity increase along the borehole to 420 m during pumping reflects the overall high transmissivities of the bedrock over this length, and indicates the penetration of shallower, less saline groundwater into and along these zones during drilling and subsequent open-hole conditions. Subsequent pumping during the electrical conductivity measurements has removed an unknown percentage of these waters and replaced them by more representative formation groundwaters of higher salinity. This effect is much less marked from 420–700 m were the overall transmissivity is lower and degree of contamination less.

Drilling consumed 626 m^3 of flushing water and the volume of returned water pumped from the borehole by air-lift pumping during drilling was 1,079 m^3. The uranine budget suggests that no flushing water has been lost to the borehole and the adjacent host bedrock during drilling. This was considered unusual but appears to be the case as subsequent sampling shows only low drilling water contents ranging from 0.21–1.8% with one anomalous value at 3.49% (see below).

Hydrochemical logging: No hydrochemical borehole logging of KLX17A has been carried out.

Comment: The measured high transmissivities relate to one or more deformation zones intercepted by KLX17A which, in turn, control the variation in salinity measured under natural and controlled conditions. Due to these high transmissive zones, which occur in the upper part of the borehole, much of the drilling water mixed with different groundwater sources (mostly from shallow to intermediate depths) have entered the rock mass from the borehole during drilling and subsequently under open hole conditions. Short circuiting therefore may be a major problem. The overall conclusion is that during open borehole conditions the groundwater/flushing water mixtures that are present in the surrounding bedrock will first have to be removed with great care before 'representative' groundwater can be accessed.

References: SKB P-07-34, P-07-164, P-07-193, P-07-221.

C2.16.1 KLX17A (416.00–437.51 m; mid. vertical elevation: –342.32 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)			x		
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)			x		
Time series (inadequate)					
Time series absent					
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)			x		
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)			x?		

Drilling Water: HLX14 (30–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KLX17A between 2006-09-13 to 2006-10-23, i.e. sample collected in 2006-11-04 and used here. Na(Ca)-HCO_3(Cl) brackish groundwater with chloride at 357 mg/L and low drilling water content (0.05%), with δ^{18}O at –11.20‰ VSMOW and δ^{2}H at –84.4‰ VSMOW; tritium at 2.5 TU, δ^{13}C at –17.20‰ PDB and ^{14}C at 49.70 pmC.

Charge Balance: Measured Sicada values given at –3.71% to +2.11%.

Time Series: 2007-03-12 to 2007-04-23 (41 days). Good time series (11 samples) show a weakly brackish, variable groundwater composition with some indication of an increase in salinity during sampling (254–591 mg/L Cl); small systematic increases in Na (195–332 mg/L), Ca (50.4–69.2 mg/L), Mg (6.0–9.8 mg/L) and SO_4 (13.70–24.40 mg/L) and decreases in HCO_3 (183–115 mg/L) are recorded. Drilling water content is consistent ranging from 0.98–1.80% during the sampling period. Complete major ions for the majority of samples.

Isotopes: Complete isotopes; δ^{13}C slightly variable at –17.10 to –16.20‰ PDB; ^{14}C variable at 41.00–52.90 pmC. Tritium (ignoring the initial value of 6.24 TU and two anomalous values of 4.32 and 4.58 TU) decreases during sampling from 2.98–1.3 TU, and δ^{18}O values at –12.50 to –14.50‰ VSMOW during the sampling period show an increasing glacial component.

Trace elements: Good coverage.

General: Na(Ca)-Cl(HCO_3) brackish glacial groundwater.

Comment: The time series data show a systematic change during the sampling period reflecting an increasing amount of groundwater of brackish glacial type; this may reflect short-circuiting in the system. Continued pumping prior to sampling should have been carried out to remove all traces of contamination caused during drilling and open hole conditions (see above). The anomalously higher tritium may reflect some contamination. Nevertheless, such brackish glacial groundwater is considered typical for such depths, and the sample chosen for Category 3 is that taken at a late stage in the sampling sequence and considered most representative.

C2.16.2 KLX17A (642.00–701.08 m; mid. vertical elevation: –547.97 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					x
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					x
Time series absent					
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					x
Major ions (incomplete)					
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HLX14 (30–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KLX17A between 2006-09-13 to 2006-10-23, i.e. sample collected in 2006-11-04 and used here. Na(Ca)-HCO_3(Cl) brackish groundwater with chloride at 357 mg/L and low drilling water content (0.05%), with $\delta^{18}O$ at –11.20‰ VSMOW and $\delta^{2}H$ at –84.4‰ VSMOW; tritium at 2.5 TU, $\delta^{13}C$ at –17.20‰ PDB and ^{14}C at 49.70 pmC.

Charge Balance: Measured Sicada values given at –3.31% to –0.037% (initial sample 11635 was omitted because > 5%).

Time Series: 2007-02-01 to 2007-02-28 (27 days). Good time series (8 samples) show a fresh groundwater stable composition (ranging from 16.8–20.1 mg/L Cl); this stability is shared by most of the other major ions although a weak decrease in HCO_3 and SO_4 is observed during the sampling period. Drilling water content (ignoring the initial sample) is consistent ranging from 0.21–0.26% during the sampling period. Complete major ions for the majority of samples.

Isotopes: Complete isotopes; $\delta^{13}C$ slightly variable at –17.00 to –16.40‰ PDB; ^{14}C variable at 50.30–52.70 pmC. Tritium (ignoring the initial value of 4.10 TU and a highly anomalous value of 32.20 TU) ranges from 1.9–3.4 TU and shows no trend during the sampling period, and $\delta^{18}O$ values constant at –10.80 to –10.90‰ VSMOW.

Trace elements: Good coverage.

General: Na-HCO_3 fresh groundwater.

Comment: The fresh groundwater sampled is not representative for this depth interval and has resulted from short circuiting pulling in such groundwater from shallower bedrock levels. This may have been facilitated by the longer than usual borehole interval sampled (about 59 m). This is further supported by the previously described groundwater sample from a shallower level being considered representative. In addition, the anomalously high tritium value of 32.20 TU is believed to be due to contamination which also introduces a question mark about the reliability of the other tritium values. Continued pumping at this level would probably not have improved the representativity of the groundwater. Allocated Category 5.

C2.17 Description of Borehole KLX18A

Borehole KLX18A is 611.28 m long (vertical depth of 602.61 m), cased to 99.93 m, and inclined at –82.10° from the horizontal. The borehole was drilled from 2006-03-29 to 2006-05-02 to better understand the geology close to the junction of the Ävrö granite and quartz monzodiorite in the central part of the Laxemar subarea, and to facilitate hydrogeological and hydrochemical investigations at depth. The dominating rock type encountered throughout the borehole consists of Ävrö granite with sporadic intercalations of varying thickness to a maximum of less than 10 m of fine-grained diorite-gabbro, and to a maximum of 15 m of diorite/gabbro. From 340–580 m, the borehole is free from these intercalations. A series of nine deformation zones characterise the borehole with a major deformation zone at about 140 m and a concentration of zones at about 360–500 m borehole length.

Differential flow logging has been carried out but no hydraulic logging or complete chemical characterisation have been conducted.

Because only one monitoring sample has been collected, no details of the differential flow logging are presented.

SKB P-06-184, P-07-98.

C2.17.1 KLX18A (472.00–489.00 m; mid. vertical elevation: –452.87 m)

Cored Borehole					
Category	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)				?	
Time series (adequate)					
Time series (inadequate)					
Time series absent				x	
Suitable section length				x	
Tube sampling					
Sampling using PLU hydraulic testing equipment					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section				x	
Hydraulic effects (short circuiting)					

Drilling Water: HLX14 (30–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KLX18A between 2006-03-29 to 2006-05-02, i.e. sample collected in 2006-11-04 and used here. Na(Ca)-HCO_3(Cl) brackish groundwater with chloride at 357 mg/L and low drilling water content (0.05%), with $\delta^{18}O$ at –11.20‰ VSMOW and δ^2H at –84.4‰ VSMOW; tritium at 2.5 TU, $\delta^{13}C$ at –17.20‰ PDB and ^{14}C at 49.70 pmC.

Charge Balance: Measured Sicada value given as –1.99%.

Time Series: Monitoring borehole section with sampling limited to one occasion in 2007-07-03. Salinity is 1,510 mg/L Cl and the drilling water content is 36.80%. Incomplete major ions: no I and TOC/DOC.

Isotopes: Incomplete isotopes; no carbon isotopes. Tritium below detection (–0.80 TU) and $\delta^{18}O$ at –14.10‰ VSMOW indicates a significant glacial component.

Trace elements: Lack of data.

General: Na(Ca)-Cl(SO_4) brackish glacial groundwater.

Comment: Brackish glacial groundwater of mainly intermediate bedrock origin. The recorded drilling water content is high and probably due to contamination from hydraulic tracer tests using uranine carried out within this borehole interval (473.3–476.3 m) on two earlier occasions: 2006-10-18 to 2006-10-29 and from 2006-10-29 to 2006-11-23. An additional major problem is the absence of time series data, incomplete major ions, no carbon isotopes and a lack of trace elements. For this depth, however, the groundwater sampled is not unusual in composition and typical of the brackish glacial groundwaters found elsewhere at intermediate depths. Allocated Category 4.

C2.18 Description of Borehole KLX19A

Borehole KLX19A (not a designated chemistry borehole) is 800.07 m long (vertical depth of 669.50 m), cased to 99.33 m, and inclined at –57.54° from the horizontal. The borehole was drilled from 2006-06-03 to 2006-09-20 with the objective of improving geological knowledge of the quartz monzodiorite (potential repository host rock) in the northwest part of the candidate area. Chemical characterisation of groundwater samples from repository depths (400–700 m) in the quartz monzodiorite was also an important objective.

The dominating rock type encountered throughout the borehole consists of quartz monzodiorite with sporadic intecalations of varying thickness (to a maximum of just under 10 m) of fine-grained granite (to a maximum of just under 30 m) of dolerite between 480–550 m, and a single minor occurrence of pegmatite at 450 m, and two intercalations of fine-grained diorite-gabbro between 690–710 m. A series of ten modelled deformation zones characterise the borehole with a concentration of 6 zones from about 410–510 m.

Differential Flow Log: Measurements carried out in borehole KLX19A from 2006-10-25 to 2006-11-22 reveal transmissivities ranging from below detection at 10^{-9} m^2s^{-1} to 10^{-4} m^2s^{-1}; higher values up to and just exceeding 10^{-6} m^2s^{-1} characterise three areas along the borehole at 140–160 m, 450–540 m and 755–780 m. The highest values occur at about 100–110 m ($10^{-4.5}$ m^2s^{-1}) and 300 m ($10^{-3.1}$ m^2s^{-1}). Lower transmissivity values (~ 10^{-9}–10^{-8} m^2s^{-1}) occur from 165 m, 210–230 m, 410 m, 670 m and 700–730 m. Under 'natural conditions' (i.e. no pumping) there is a clear subdivision between natural flow from the bedrock to the borehole from 100–220 m with flow rates mostly between 10^1–$10^{4.1}$ mL h^{-1}, and from the borehole out into the surrounding bedrock at 300 m with a flow rate of $10^{4.3}$ mL h^{-1} and from about 450–520 m and 670–780 m with flow rates of about 10^1–10^3 mL h^{-1}. With pumping, all groundwater flow is reversed towards the borehole at flow rates of $10^{1.6}$–$10^{4.4}$ mL h^{-1}, including some additional groundwaters from about 410 m with a flow rate of 10^2 mL h^{-1}.

Pump tests carried out during drilling show that the most transmissive section is from 102–197 m, in accordance with the differential flow log measurements.

Electrical Conductivity log: The hydraulic complexity of the open borehole conditions is further supported by the electrical conductivity log. Under 'natural' open hole conditions (i.e. no pumping), a fairly uniform salinity (~ 0.08–0.09 Sm^{-1}) is indicated from 100–350 m, whereupon a slight but systematic increase occurs down to the bottom of the borehole at about 0.15 Sm^{-1}. During the pumping stage the salinity level increases forming a step-wise pattern with depth, from 110–300 (0.2 Sm^{-1}) and 300–510 (0.3–0.4 Sm^{-1}), and then a more uniform increase (from 0.4–1.3 Sm^{-1}) to the bottom of the borehole.

The removal during pumping of the shallower, less saline groundwater which had penetrated into the more transmissive parts of the borehole during drilling and subsequent open-hole conditions, especially in the intermediate to shallow parts of the borehole, may or may not have achieved the representative formation groundwater salinities. At depths greater than 500 m, where the bedrock transmissivities are lower (and also the formation groundwaters are more saline), less penetration of more shallow-derived less saline waters has occurred, and pumping may have been more efficient in removing contaminated water. Waters collected at depth therefore may be more representative of the formation groundwaters.

Hydrochemical logging: Measurements in the borehole were carried out in 2006-10-18, only one week prior to the differential flow measurements. As a result, the hydrochemical logging showed a similar pattern and general range of electrical conductivity values with constant salinity to about 400 m followed by a gradual increase to 700 m; in contrast to the differential flow log, a sharp increase in salinity was recorded at the borehole bottom. The amount of drilling water in the borehole during hydrochemical logging was significant, ranging from 5.72–6.98% to about 300 m followed by an increase to 12.90% at 400 m, and then a more rapid increase to 67.7% at 800 m. The total variation in chloride along the borehole is 93.7–113 mg/L to 400 m followed by an increase to 301 at 700 m and finally a sharp increase to 867 mg/L at 800 m,. i.e. generally a brackish type groundwater mix.

Comment: The measured high transmissivities relate to the several deformation zones intercepted by KLX19A which, in turn, control the variation in salinity measured under natural and controlled conditions. Due to the high transmissive deformation zones, much of this drilling water mixed with different groundwater sources (mostly from shallow to intermediate depths) have entered the rock mass from the borehole during drilling and subsequently under open hole conditions. These waters will first have to be removed with great care before 'representative' groundwater can be accessed. Short circuiting therefore may be a major problem.

References: SKB P-06-310, P-07-20, P-07-90, P-07-202.

C2.18.1 KLX19A (40.00–90.00 m; mid. vertical elevation: –38.02 m)

Cored Borehole					
Category	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)				x	
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent				x	
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling				x	
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Drilling Water: HLX28 (6.03–154.20 m borehole length; mid. vertical elevation: –52.67 m). There are three documented drilling water samples used during drilling in the Extended L.2.3 dataset and these show good stability. Sample used here was collected in 2005-04-12 and chosen over the other earlier and later samples because it included isotope values. Na-HCO_3 type fresh groundwater with low chloride (39.3 mg/L) and $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –76.5‰ VSMOW; tritium at 1 TU, $\delta^{13}C$ at –16.15‰ PDB and ^{14}C at 46.91 pmC.

Charge Balance: Measured Sicada value given at –1.49%.

Time Series: Only one sample taken using tube sampling in 2006-10-18 (initial sample). Groundwater is fresh (96.9 mg/L Cl) with a drilling water content of 6.9%. Major ions incomplete, no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Incomplete isotopes; no carbon isotopes. Tritium at 2.7 TU and $\delta^{18}O$ at –11.30‰ VSMOW.

Trace elements: Lack of data.

General: Na(Ca)-HCO_3(Cl) fresh groundwater.

Comment: Despite the tube sample, and the absence of time series, incomplete major ions and isotope data, no trace element data and high drilling water (perhaps contamination), the borehole section is reasonably constrained and the stability of the near-surface groundwater chemistry tends to be more predictable, therefore reflecting that expected at these shallow depths. Allocated Category 4.

C2.18.2 KLX19A (499.0–519.00 m; mid. vertical elevation: –410.52 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					x
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					x
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					x
Major ions (incomplete)					
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					
Monitoring borehole section					x
Hydraulic effects (short circuiting)					?

Drilling Water: HLX28 (6.03–154.20 m borehole length; mid. vertical elevation: –52.67 m). There are three documented drilling water samples used during drilling in the Extended L.2.3 dataset and these show good stability. Sample used here was collected in 2005-04-12 and chosen over the other earlier and later samples because it included isotope values. Na-HCO_3 type fresh groundwater with low chloride (39.3 mg/L) and $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –76.5‰ VSMOW; tritium at 1 TU, $\delta^{13}C$ at –16.15‰ PDB and ^{14}C at 46.91 pmC.

Charge Balance: Measured Sicada value given as –4.49%.

Time Series: Monitoring borehole section with sampling limited to one occasion in 2007-01-08; salinity is 1,780 mg/L Cl and the drilling water content is 7.5%. Complete major ions.

Isotopes: Complete isotopes; $\delta^{13}C$ at –15.10‰ PDB; ^{14}C at 29.88 pmC. Tritium at 1.8 TU, and $\delta^{18}O$ at –13.80‰ VSMOW indicate a significant glacial component.

Trace elements: Good coverage.

General: Na(Ca)-Cl(SO_4) brackish glacial groundwater.

Comment: Brackish glacial groundwater of mainly intermediate bedrock origin. A major problem is the absence of time series data and presence of significant drilling water. For this depth, however, the groundwater sampled is not unusual in composition, and typical of the brackish glacial groundwaters found elsewhere at intermediate depths. Nevertheless, Category 5 allocated.

C2.18.3 KLX19A (509.0–517.00 m; mid. vertical elevation: –413.86 m)

Cored Borehole Category	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)			x		
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)			x		
Time series absent					
Suitable section length			x		
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)			x		
Environmental isotopes (incomplete)					
Monitoring borehole section			x		
Hydraulic effects (short circuiting)			x?		

Drilling Water: HLX28 (6.03–154.20 m borehole length; mid. vertical elevation: –52.67 m). There are three documented drilling water samples used during drilling in the Extended L.2.3 dataset and these show good stability. Sample used here was collected in 2005-04-12 and chosen over the other earlier and later samples because it included isotope values. Na-HCO_3 type fresh groundwater with low chloride (39.3 mg/L) and $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –76.5‰ VSMOW; tritium at 1 TU, $\delta^{13}C$ at –16.15‰ PDB and ^{14}C at 46.91 pmC.

Charge Balance: Measured Sicada values given as –2.24 to –0.75%.

Time Series: Monitoring borehole section sampled on three occasions in 2007-06-13, 2007-07-04 and 2007-08-21; salinity increases from 699–1,750 mg/L Cl accompanied by increases in Na (450–962 mg(L), Ca (56.70–152.00 mg/L) and SO_4 (84.40–122.00 mg/L), and decreases in HCO_3 (149.0–36.3 mg/L). the drilling water content during the three sampling periods was 12.7% to 14.8% to 6.9%. Complete major ions for the first and third sampling occasions; no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC for the second sampling.

Isotopes: Complete isotopes for the first and third sampling occasions; $\delta^{13}C$ at –16.70 and –17.80‰ PDB; ^{14}C at 43.00 and 31.00 pmC. Tritium at 1.8 TU and under detection for the third sample (–0.8 TU); $\delta^{18}O$ values at –12.10 and –13.90‰ VSMOW indicating an increased glacial component with time.

Trace elements: Good coverage for the first and second sampling occasions; second occasion there is a lack of data.

General: Na(Ca)-Cl(SO_4) brackish glacial groundwater.

Comment: Brackish glacial groundwater of mainly intermediate bedrock origin. There is a clear change to greater groundwater mineralisation with time (possibly indicating some short circuiting), accompanied by a decrease in tritium to under detection and a decrease of pmC. In fact, the groundwater composition on the third occasion is very similar to the previous sample described from almost the same borehole location some 5–6 months earlier. The first two sampling occasions have simply removed contaminated water since the installation of the monitoring equipment. The decrease in drilling water during the three sampling occasions does not appear to be influenced by anthropogenic contamination from tracer flow tests; none were carried out in KLX19A or in the near-vicinity boreholes. Category 3 allocated to the latest sample collected.

C2.18.4 KLX19A (764.00–769.00 m; mid. vertical elevation: –624.78 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)				x	
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent				x	
Suitable section length				x	
Sampling during drilling					
Sampling using PLU hydraulic testing equipment				x	
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)				x	
Major ions (incomplete)					
Environmental isotopes (complete)				x	
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HLX28 (6.03–154.20 m borehole length; mid. vertical elevation: –52.67 m). There are three documented drilling water samples used during drilling in the Extended L.2.3 dataset and these show good stability. Sample used here was collected in 2005-04-12 and chosen over the other earlier and later samples because it included isotope values. Na-HCO_3 type fresh groundwater with low chloride (39.3 mg/L) and $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –76.5‰ VSMOW; tritium at 1 TU, $\delta^{13}C$ at –16.15‰ PDB and ^{14}C at 46.91 pmC.

Charge Balance: Measured Sicada value given at –2.07%.

Time Series: Only one sample taken using the PLU hydraulic testing equipment in 2006-12-05. Groundwater is brackish (3,520 mg/L Cl) with a drilling water content of 7.047%. Complete major ions.

Isotopes: Complete isotopes; $\delta^{13}C$ at –15.85‰ PDB; ^{14}C at 46.76 pmC. Tritium at 1.5 TU, and $\delta^{18}O$ at –12.7‰ VSMOW indicates a weak glacial component.

Trace elements: Good coverage.

General: Na(Ca)-Cl(SO_4) brackish groundwater.

Comment: Brackish groundwater with a weak glacial component. Major problem is the absence of time series data and high drilling water content. For this depth, however, the groundwater sampled is not unusual in composition, and fairly typical of the brackish groundwaters found elsewhere at intermediate depths. Category 4 allocated.

KLX19A: Tube samples sampled every 50 m from 140.00–790.00 m (2006-10-18) are considered unrepresentative and allocated Category 5.

C2.19 Description of Borehole KLX20A

Borehole KLX20A is 475.92 m long (vertical depth of 338.58 m), cased to 99.91 m, and inclined at –50.02° from the horizontal. The borehole was drilled from 2006-03-25 to 2006-04-24 and the main objectives were: a) to drill through and characterise the NS001 deformation zone, b) to provide further information of the rock properties in the quartz monzodiorite which is the dominating rock type in the southwestern part of the Laxemar subarea, and c) to facilitate hydrogeological and hydrochemical investigations at depth. The dominating rock type encountered throughout the borehole consists of quartz monzodiorite with one major intercalation of dolerite at about 180–230 m and minor sporadic intercalations of fine-grained granite (metre scale) in the upper 180 m and one fine-grained diorite-gabbro (~ 10 m) at 390–400 m depth. A series of four deformation zones generally characterise the borehole with a major deformation zone at about 170–230 m borehoe length.

Differential flow logging, hydraulic injection tests and hydraulic logging have been conducted.

Because only one monitoring sample has been collected, no details of the differential flow logging and hydrochemical logging are presented.

SKB P-06-181, P-06-183, P-06-312, P-07-49, P-07-134.

C2.19.1 KLX20A (0.00–50.00 m; mid. vertical elevation: –8.08.02 m)

Cored Borehole					
Category	**1**	**2**	**3**	**4**	**5**
Drilling water (≤ 1%)					
Drilling water (≤ 5%)				x	
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent				x	
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling				x	
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Drilling Water: HLX28 (6.03–154.20 m borehole length; mid. vertical elevation: –52.67 m). There are three documented drilling water samples used during drilling in the Extended L.2.3 dataset and these show good stability. Sample used here was collected in 2005-04-12 and chosen over the other earlier and later samples because it included isotope values. Na-HCO$_3$ type fresh groundwater with low chloride (39.3 mg/L) and δ^{18}O at –10.9‰ VSMOW and δ^{2}H at –76.5‰ VSMOW; tritium at 1 TU, δ^{13}C at –16.15‰ PDB and ^{14}C at 46.91 pmC.

Charge Balance: Measured Sicada value given at –0.83%.

Time Series: Only one sample taken using tube sampling in 2006-06-14 (initial sample). Groundwater is fresh (15 mg/L Cl) with a drilling water content of 1.27%. Major ions incomplete, no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Incomplete isotopes; no carbon isotopes. Tritium at 2.5 TU and $\delta^{18}O$ at –11.90‰ VSMOW.

Trace elements: Lack of data.

General: Na-HCO_3(Cl) fresh groundwater.

Comment: Despite the tube sample, and the absence of time series, incomplete major ions and isotope data, no trace element data and some drilling water, the borehole section is reasonably constrained and the stability of the near-surface groundwater chemistry tends to be more predictable, therefore reflecting that expected at these shallow depths. Allocated Category 4.

KLX20A: Tube samples sampled every 50 m from 100.00–425.00 m (2006-06-14) are considered unrepresentative and allocated Category 5.

C2.20 Description of Borehole KLX21B

Borehole KLX21B is 858.78 m long (vertical depth of 800.04 m), cased to 100.58 m, and inclined at –70.85° from the horizontal. The borehole was drilled from 2006-10-12 to 2006-11-29 to better understand the geology in the eastern part of the Laxemar subarea and to facilitate hydrogeological and hydrochemical investigations at depth. The dominating rock type encountered throughout the borehole consists of Ävrö granite with sporadic intercalations of fine-grained dioritoid varying thickness from a few metres to a maximum of about 30 m. Sporadic intercalations of fine-grained granite occur doen to about 500 m borehole length. The final part of the borehole from 770–859 m borehole length is dominantly of quartz monzodiorite with minor intercalations of Ävrö granite. A series of nine deformation zones generally characterise the borehole with a major deformation zone at about 600–700 m.

Differential flow logging and hydraulic logging have been conducted.

Because only one monitoring sample has been collected, no details of the differential flow logging and hydrochemical logging are presented.

SKB P-06-184, P-07-73, P-07-98, P-07-189, P-08-24.

6.2.20.1 KLX21B (0.00–40.00 m; mid. vertical elevation: –8.20 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)				x	
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent				x	
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling				x	
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Drilling Water: HLX10 (3.00–85.00 m borehole length; mid. vertical elevation: –29.25 m). There are three documented drilling water samples used during the drilling of KLX21B in the Extended L.2.3 dataset and these show good stability. Sample used here is the most recent collected in 2005-10-28. Na-HCO_3 type fresh groundwater with low chloride (31.9 mg/L) and $\delta^{18}O$ at –10.8‰ VSMOW and $\delta^{2}H$ at –76.9‰ VSMOW; tritium at 5.7 TU, $\delta^{13}C$ at –16.12‰ PDB and ^{14}C at 52.73 pmC.

Charge Balance: Measured Sicada value given at +4.32%.

Time Series: Only one sample taken using tube sampling in 2007-01-09 (initial sample). Groundwater is fresh (51.3 mg/L Cl) with a drilling water content of 1.57%. Major ions incomplete, no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Isotopes: Incomplete isotopes; no carbon isotopes Tritium at 4.4 TU and $\delta^{18}O$ at –11.10‰ VSMOW.

Trace elements: Lack of data.

General: Na(Ca)-HCO_3(Cl,SO_4) fresh groundwater.

Comment: Despite the tube sample, and the absence of time series, incomplete major ions and isotope data, no trace element data and some drilling water, the borehole section is reasonably constrained and the stability of the near-surface groundwater chemistry tends to be more predictable, therefore reflecting that expected at these shallow depths. Short circuiting cannot be ruled out. Allocated Category 4.

KLX21B: Tube samples sampled every 50 m from 90.00–840.00 m (2007-01-09) are considered unrepresentative and allocated Category 5.

Appendix D

Simpevarp data

Details of the Simpevarp borehole drilling are given in SKB P-03-113 (KSH01A), SKB P-04-15 (KSH02) and SKB P-04-233 (KSH03A), and the quality assurance approach used to evaluate the Simpevarp percussion and cored boreholes is given in SKB R-04-16 and SKB R-04-74 and will not be repeated here. Presented are the updated data in terms of categorisation following the procedure outlined in section 3.1 and used throughout this documentation. In addition, a brief description of each cored borehole is given.

D1 Percussion boreholes

D1.1 HSH02 (0.00–200.00 m; mid. vertical elevation: –90.53 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					
Section without flow log (0–200 m)			x		
Time series/monitoring			x		
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)			x		
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)			x?		

Charge Balance: Measured Sicada values given at –0.07% to +1.14%.

Time Series: Sampled on 5 occasions from 2003-01-31 to 2003-08-27 (~ 3 months). Adequate time series (5 samples) showing variable salinity (7.0–22.6 mg/L Cl); variability reflected also by the other major ions. Incomplete major ions; no I, S^{2-}, Fe^{2+} and DOC.

Isotopes: Complete isotopes for the first two sampling occasions; $\delta^{13}C$ at –17.30 to –16.90‰ PDB, ^{14}C at 67.28–69.84 pmC. Tritium variable at 11.0–15.3 TU and $\delta^{18}O$ at –10.8 to –10.7‰ VSMOW. Other sampled occasions show similar ranges for tritium and $\delta^{18}O$.

Trace elements: Lack of data.

General: Na-HCO_3 fresh meteoric water of modern recharge character.

Comment: Limited time series, incomplete major elements and absence of trace element data, coupled with a long 100 m borehole length (facilitating mixing/short circuiting). However, such a groundwater composition is expected at such shallow depths. Category 3 allocated to the second sampled groundwater.

D1.2 HSH03 (0.00–103.00 m; mid. vertical elevation: –48.11 m)

Percussion Borehole Category	1	2	3	4	5
Short restricted section length					
Section with flow log					
Section without flow log (0–50 m)					
Section without flow log (0–100 m)					
Section without flow log (0–200 m)				x	
Time series/monitoring				x	
Time series absent					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Charge Balance: Measured Sicada values given at –4.60% to +1.56%.

Time Series: Sampled on 5 occasions from 2002-08-2 to 2004-02-06 (~ 1.8 years). Adequate time series (5 samples) showing marked increase in salinity with time (55.1–949.0 mg/L Cl); increase also indicated by Na, K, Ca and Mg, and a decrease in HCO_3; SO_4 is variable but overall an increase. Small amount of drilling water recorded at 0.03%. Incomplete major ions; no I, S^{2-}, Fe^{2+} and DOC.

Isotopes: Complete isotopes for the final two sampling occasions; $\delta^{13}C$ at –17.80 to –16.90‰ PDB, ^{14}C at 59.30–61.00 pmC. Tritium variable at 4.7–10.0 TU and $\delta^{18}O$ at –10.8 to –10.4‰ VSMOW. Other sampled occasions show similar ranges for tritium and $\delta^{18}O$.

Trace elements: Lack of data.

General: Na-HCO_3 to Na(Ca)-Cl(HCO_3,SO_4) transition from fresh to brackish groundwater type with time.

Comment: Major problem is the clear transition from a fresh to a brackish groundwater. The fresh meteoric modern recharge type has been selected as the more likely groundwater at this depth. Also, lack of some major elements and absence of trace element data, coupled with a long 103 m borehole length (facilitating mixing/short circuiting). However, as indicated, such a groundwater composition is expected at such shallow depths. Category 4 allocated to the initial sampled groundwater.

D2 Cored boreholes

D2.1 Description of Borehole KSH01A

Borehole KSH01A is 1,003.00 m long (vertical depth of 968.43 m), cased to 100.28 m, and inclined at –80.44° from the horizontal. The borehole was drilled from 2002-8-22 to 2003-12-18 and the main objectives were to gain geological information at depth of the eastern part of the Simpevarp peninsula and to facilitate hydrogeological and hydrochemical investigations at this depth. Borehole KSH01A penetrates different rock units. The main rock type in the upper part of the borehole (to 345 m) is the quartz monzodiorite with smaller volumes of dioritoid at 205–245 m and 325–340 m; larger amounts of dioritoid occur from 345–630 m. At greater depths to 1,000 m are found granitic to granodioritic rocks (Ävrö granite) mixed with quartz monzodiorite. Smaller horizons of fine-grained granite occur at 360–365 m (mixed with pegmatite), 680–690 m and 720–730 m (mixed with mafic rocks) and 860–870 m. Large lengths of the drillcore show an increased fracture frequency accompanied by intense wall rock alteration/oxidation. This is most prominent in sections 250–285 m, 420–450 m and 590–630 m. Below 700 m the fracture frequency is significantly lower and only a slight alteration of the rock is observed.

References: SKB P-03-70, P-03-87, P-03-113, P-04-32, R-04-16, R-04-74. Discussion of the differential flow logging and hydrochemical logging data and their interpretation are presented in R-04-16 and R-04-74.

D2.1.1 KSH01A (156.50–167.00 m; mid. vertical elevation: –152.74 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)		x			
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)		x			
Time series (inadequate)					
Time series absent					
Suitable section length		x			
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)		x			
Major ions (complete)		x			
Major ions (incomplete)					
Environmental isotopes (complete)		x			
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)		x?			

Drilling Water: HSH03 (0.00–103.00 m). There is one documented sample from the time of drilling borehole KSH01A (to 1,003 m from 2002-08-22 to 2003-01-17); in the Extended L.2.3 dataset the documented sample is from the first day of drilling and used here. Na-HCO_3 fresh meteoric groundwater with low chloride (55.1 mg/L). Tritium at 10.0 TU, $\delta^{18}O$ at –10.7‰ VSMOW and δ^2H at –76.1‰ VSMOW.

Charge Balance: Measured Sicada values at –1.76% to –0.33%.

Time Series: Sampled from 2003-03-31 to 2003-04-22 (22 days) with a reasonable time series (6 occasions). Brackish groundwater showing a systematic increase with time (5,166–5,590 mg/L Cl), reflected by increases in Na, K and Ca and decreases in HCO_3 and SO_4; Mg shows no obvious trend. More time series desired. Drilling water decreases systematically from 3.70–2.39% during the sampling occasion. Major ions complete.

Trace elements: Good coverage.

Isotopes: Complete for three sampling occasions; ^{14}C at ~ 30 pmC, $\delta^{13}C$ at ~ –19.00‰ PDB. Tritium below detection (–0.8 TU) apart from the first sample at 2.8 TU, and $\delta^{18}O$ showing a small depletion with time (–12.70 to –13.01‰ VSMOW) indicating an increasing but weak glacial component.

General: Na(Ca)-Cl brackish non-marine groundwater with a small marine component (~ 71 mg/L Mg) and a weak glacial component.

Comment: Unstable groundwater with a decreasing drilling water component and a systematic change with most major ions during the sampling period. Additional time series data would have been useful. Nevertheless, the final sample is considered close to being representative for this depth. Allocated Category 2.

D2.1.2 KSH01A (197.00–313.42 m; mid. vertical elevation: –243.59 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)				–	
Drilling water (≤ 5%)				–	
Drilling water (≤ 10%)				–	
Drilling water (> 10%)				–	
Time series (adequate)					
Time series (inadequate)					
Time series absent				x	
Suitable section length					
Tube sampling					
Sampling during drilling				x	
Sampling using PLU hydraulic testing equipment					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)				x	
Major ions (incomplete)					
Environmental isotopes (complete)				x	
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)				x?	

Drilling Water: HSH03 (0.00–103.00 m). There is one documented sample from the time of drilling borehole KSH01A (to 1,003 m from 2002-08-22 to 2003-01-17); in the Extended L.2.3 dataset the documented sample is from the first day of drilling and used here. Na-HCO_3 fresh meteoric groundwater with low chloride (55.1 mg/L). Tritium at 10.0 TU, $\delta^{18}O$ at –10.7‰ VSMOW and $\delta^{2}H$ at –76.1‰ VSMOW.

Charge Balance: Measured Sicada value at +2.11%.

Time Series: Section sampled during drilling on one occasion (2002-10-24). Brackish groundwater (5,982 mg/L Cl) with significant Mg (61.2 mg/L); drilling water not recorded. Major ions incomplete, no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC.

Trace elements: Lack of data.

Isotopes: Complete; $\delta^{13}C$ at –21.42‰ PDB, ^{14}C at 36.35 pmC. Tritium at 1.10 TU, and $\delta^{18}O$ at –14.10‰ VSMOW indicates a significant glacial component.

General: Na(Ca)-Cl brackish non-marine groundwater with glacial and marine components.

Comment: Generally a brackish non-marine groundwater with a weak marine component and a significant glacial component. The problem is an absence of time series and a long borehole section (116 m) that may have facilitated mixing/short circuiting. Also no recorded drilling water and incomplete major ions. Nevertheless, at these depths groundwater mixtures are to be expected. Allocated Category 4.

D2.1.3 KSH01A (245.00–261.58 m; mid. vertical elevation: –241.72 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)			x		
Drilling water (> 10%)					
Time series (adequate)			x		
Time series (inadequate)					
Time series absent					
Suitable section length			x		
Tube sampling					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)			x		
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HSH03 (0.00–103.00 m). There is one documented sample from the time of drilling borehole KSH01A (to 1,003 m from 2002-08-22 to 2003-01-17); in the Extended L.2.3 dataset the documented sample is from the first day of drilling and used here. Na-HCO_3 fresh meteoric groundwater with low chloride (55.1 mg/L). Tritium at 10.0 TU, $\delta^{18}O$ at –10.7‰ VSMOW and $\delta^{2}H$ at –76.1‰ VSMOW.

Charge Balance: Measured Sicada values at –2.95% to –1.13%.

Time Series: Sampled from 2003-04-29 to 2003-05-15 (16 days) with a reasonable time series (5 occasions). Brackish groundwater showing good saline stability (6,298–6,342 mg/L Cl) reflected by the other major ions. Drilling water consistent at 7.48–8.22% during the sampling occasion. Major ions complete.

Trace elements: Good coverage.

Isotopes: Complete; no carbon isotopes (lack of $HCO_3 < 20$ mg/L). Tritium below detection (–0.8 TU) and $\delta^{18}O$ at –14.00 to –13.30‰ VSMOW) indicating a significant glacial component.

General: Na(Ca)-Cl brackish non-marine groundwater with a small marine component (~ 64 mg/L Mg) and a significant glacial component.

Comment: Good representative groundwater from this depth; main negative property is the persistent high drilling water content. Allocated Category 3.

D2.1.4 KSH01A (238.00–277.00 m; mid. vertical elevation: –243.59 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)			?		
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)			x		
Time series absent					
Suitable section length					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Tube sampling					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)			x		
Environmental isotopes (incomplete)					
Monitoring borehole section			x		
Hydraulic effects (short circuiting)			x?		

Drilling Water: HSH03 (0.00–103.00 m). There is one documented sample from the time of drilling borehole KSH01A (to 1,003 m from 2002-08-22 to 2003-01-17); in the Extended L.2.3 dataset the documented sample is from the first day of drilling and used here. Na-HCO_3 fresh meteoric groundwater with low chloride (55.1 mg/L). Tritium at 10.0 TU, $\delta^{18}O$ at –10.7‰ VSMOW and δ^2H at –76.1‰.

Charge Balance: Measured Sicada values at +0.20% to –4.12% (first sample at +10.01% omitted).

Time Series: Sampled on three occasions (2005-11-15, 2006-06-30 and 2006-11-08) from a monitoring borehole; reasonable time series. Brackish groundwater showing some instability (decrease) in salinity (6,320–6,570 mg/L Cl) reflected by decreases in Na, K, Ca and SO_4, but showing a small increase in Mg (to 68.7 mg/L). Drilling water not recorded during the first sampling period; the other two occasions show a decrease in drilling water from 6.61 to 4.32%. Major ions complete for the selected sample during the second sampling period; otherwise no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC in the final sample.

Trace elements: Good coverage for the selected sample.

Isotopes: Complete; no carbon isotopes (lack of HCO_3 ~ 20 mg/L). Tritium below detection (–0.8 TU) for the selected sample (otherwise a small increase to 1.8 TU in the final sample), and $\delta^{18}O$ at –13.70 to –13.30‰ VSMOW indicating a significant glacial component.

General: Na(Ca)-Cl brackish non-marine groundwater with a small marine component (~ 62.5 mg/L Mg) and a significant glacial component.

Comment: Good representative groundwater from this depth (compare previous sample from almost the same depth); main negative property is the lack of time series, the drilling water content and a somewhat long borehole section (39 m) which may have facilitated some mixing/short circuiting. With respect to the drilling water, this section was subject to hydraulic tracer tests using uranine from 2005-11-29 to 2005-12-07, and therefore the drilling water contents in the last two sampling periods may have been influenced by residual uranine in the system during groundwater sampling. Allocated Category 3.

D2.1.5 KSH01A (532.00–572.00 m; mid. vertical elevation: –531.51 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)			?		
Drilling water (> 10%)					
Time series (adequate)			x		
Time series (inadequate)					
Time series absent					
Suitable section length					
Tube sampling					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)			x		
Major ions (incomplete)					
Environmental isotopes (complete)			x		
Environmental isotopes (incomplete)					
Monitoring borehole section			x		
Hydraulic effects (short circuiting)			x?		

Drilling Water: HSH03 (0.00–103.00 m). There is one documented sample from the time of drilling borehole KSH01A (to 1,003 m from 2002-08-22 to 2003-01-17); in the Extended L.2.3 dataset the documented sample is from the first day of drilling and used here. Na-HCO$_3$ fresh groundwater with low chloride (55.1 mg/L). Tritium at 10.0 TU, δ^{18}O at –10.7‰ VSMOW and δ^{2}H at –76.1‰ VSMOW.

Charge Balance: Measured Sicada values at –2.64% to +0.43%.

Time Series: Sampled on three occasions (2005-11-18, 2006-06-20 and 2006-11-09) from a monitoring borehole; reasonable time series. Brackish groundwater showing instability (increase) in salinity (8,440–9,130 mg/L Cl) reflected by increases in Na and Ca; K, Mg and SO$_4$ show no trend. Drilling water is high at 12.50%, 17.50% to 9.27% with increasing time. Major ions complete for the selected sample during the second sampling period; otherwise no Fe(tot), Fe^{2+}, S^{2-} and TOC/DOC for the other two sampling occasions.

Trace elements: Good coverage for the selected sample.

Isotopes: Complete; no carbon isotopes (lack of HCO$_3$ ~ 20 mg/L). Tritium below detection (–0.8 TU) for the last two samples (otherwise a small increase to 1.7 TU in the initial sample), and δ^{18}O at –12.60 to –12.40‰ VSMOW suggesting a weak glacial component.

General: Na(Ca)-Cl brackish non-marine groundwater with a small marine component (~ 40 mg/L Mg) and a weak glacial component.

Comment: Good representative groundwater from this increased depth level with greater salinity and diminished components of marine and glacial waters; main negative property is the lack of time series, the drilling water content and a somewhat long borehole section (40 m) which may have facilitated some mixing/short circuiting. With respect to the drilling water, this section was subject to hydraulic tracer tests using uranine from 2005-11-29 to 2005-12-07, and therefore the drilling water contents in the last two sampling periods may have been influenced by residual uranine in the system during groundwater sampling. Allocated Category 3.

D2.1.6 KSH01A (548.00–565.35 m; mid. vertical elevation: –536.04 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)			x		
Time series (adequate)					
Time series (inadequate)			x		
Time series absent					
Suitable section length					
Tube sampling					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment			x		
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)			x		
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HSH03 (0.00–103.00 m). There is one documented sample from the time of drilling borehole KSH01A (to 1,003 m from 2002-08-22 to 2003-01-17); in the Extended L.2.3 dataset the documented sample is from the first day of drilling and used here. Na-HCO$_3$ fresh meteoric groundwater with low chloride (55.1 mg/L). Tritium at 10.0 TU, δ^{18}O at –10.7‰ VSMOW and δ^{2}H at –76.1‰ VSMOW.

Charge Balance: Measured Sicada values at –0.14% to +0.30%.

Time Series: Sampled on two occasions (2003-08-21 and 2003-09-15) using the PLU hydraulic testing equipment; inadequate time series. Brackish groundwater showing stability in salinity (8,755–8,875 mg/L Cl) generally reflected by the other major ions. Drilling water is high showing a decrease from 13.45% to 10.74%, with increasing time. Incomplete major ions; no Fe(tot), Fe^{2+}, S^{2-}, I, and TOC/DOC.

Trace elements: Good coverage for the selected sample.

Isotopes: Complete; no carbon isotopes (lack of HCO$_3$ ~ 12 mg/L). Tritium at 2.0–1.1 TU and δ^{18}O at –12.70 to –12.60‰ VSMOW.

General: Na(Ca)-Cl(SO$_4$) brackish non-marine groundwater similar to the previous sample in that there is a decrease in the marine (~ 40 mg/L Mg) and glacial components compared to the shallower samples around 250 m depth.

Comment: Good representative groundwater from this increased depth level with greater salinity and unchanged components of marine and glacial waters; main negative properties are the lack of time series and the high drilling water contents. Allocated Category 3.

D2.1.7 KSH01A (531.00–619.52 m; mid. vertical elevation: –554.01 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					x
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					
Tube sampling					
Sampling during drilling					x
Sampling using PLU hydraulic testing equipment					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HSH03 (0.00–103.00 m). There is one documented sample from the time of drilling borehole KSH01A (to 1,003 m from 2002-08-22 to 2003-01-17); in the Extended L.2.3 dataset the documented sample is from the first day of drilling and used here. Na-HCO_3 fresh meteoric groundwater with low chloride (55.1 mg/L). Tritium at 10.0 TU, $\delta^{18}O$ at –10.7‰ VSMOW and $\delta^{2}H$ at –76.1‰ VSMOW.

Charge Balance: Measured Sicada value at –0.13%.

Time Series: Sampled on one occasion (2002-11-20) during drilling; time series absent. Brackish groundwater with a salinity of 3,922 mg/L Cl. Drilling water is high at 34.98%. Incomplete major ions; no Fe(tot), Fe^{2+}, S^{2-}, I, and TOC/DOC.

Trace elements: Lack of data.

Isotopes: Complete; $\delta^{13}C$ at –15.70‰ PDB, ^{14}C at 57.08 pmC. Tritium at 4.2 TU and $\delta^{18}O$ at –10.70‰ VSMOW.

General: Na(Ca)-Cl(SO_4) brackish groundwater mix with a small marine (~ 42 mg/L Mg) component.

Comment: Compared to the previous samples at these intermediate depths, this sample is not representative. Problems include high drilling water content, contamination during drilling and a long borehole section (88.52 m) probably facilitating mixing/short circuiting. Allocated Category 5.

D2.1.8 KSH01A (585.00–593.00 m; mid. vertical elevation: –567.37 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					x
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					x
Tube sampling					
Sampling during drilling					x
Sampling using PLU hydraulic testing equipment					
Charge balance ±5% (±10% for <50 mg/L Cl)					x
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					x
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					x?

Drilling Water: HSH03 (0.00–103.00 m). There is one documented sample from the time of drilling borehole KSH01A (to 1,003 m from 2002-08-22 to 2003-01-17); in the Extended L.2.3 dataset the documented sample is from the first day of drilling and used here. Na-HCO_3 fresh meteoric groundwater with low chloride (55.1 mg/L). Tritium at 10.0 TU, $\delta^{18}O$ at –10.7‰ VSMOW and $\delta^{2}H$ at –76.1‰ VSMOW.

Charge Balance: Measured Sicada value at –0.11%.

Time Series: Sampled on one occasion (2002-11-16) during drilling. Brackish groundwater with a salinity of 1,298.6 mg/L Cl. Drilling water is high at 66.09%. Incomplete major ions; no Fe(tot), Fe^{2+}, S^{2-}, I, and TOC/DOC.

Trace elements: Lack of data.

Isotopes: Complete; $\delta^{13}C$ at –16.30‰ PDB, ^{14}C at 59.81 pmC. Tritium at 6.2 TU and $\delta^{18}O$ at –10.60‰ VSMOW.

General: Na(Ca)-Cl(SO_4,SO_4) brackish groundwater mix.

Comment: Compared to the previous samples at these intermediate depths, this sample is not representative. Problems include high drilling water content, contamination during drilling. Allocated Category 5.

KSH01A: Tube samples sampled every 50 m from 50.00–1,000.00 m (2003-01-29) are considered unrepresentative and allocated Category 5.

D2.2 Description of Borehole KSH02

Borehole KSH02 is 1,001.11 m long (vertical depth of 999.43 m), cased to 100.26 m, and inclined at –85.70° from the horizontal. The borehole was drilled from 2002-01-22 to 2003-06-11 and the main objectives were gain geological information at depth of the central part of the Simpevarp peninsula and to facilitate hydrogeological and hydrochemical investigations at this depth. Borehole KSH02, in comparison to KSH01A, penetrates a relatively homogeneous rock mass dominated by fine-grained dioritoid. Between about 500–750 m there is an increase in thin intercalations of fine-grained granite and subsidiary pegmatite; only one significant horizon of fine-grained diorite-gabbro occurs close to the bottom of the borehole. Large lengths of the drill-core to 800 m show an increased fracture frequency (6–10 open fractures/metre) accompanied by intense wall rock alteration/oxidation. This is most prominent in sections 280–310 m and 450–650 m. Below 750 m the fracture frequency is significantly lower (1–4 open fractures/metre) and only a slight alteration of the rock is observed.

References: SKB P-03-88, P-03-110, P-04-151, P-04-247, P-04-281, P-04-289, R-04-16, R-04-74. Discussion of the differential flow logging and hydrochemical logging data and their interpretation are presented in R-04-16 and R-04-74.

D2.2.1 KSH02 (419.00–424.00 m; mid. vertical elevation: –415.17 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)			x		
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)			x		
Time series absent					
Suitable section length			x		
Tube sampling					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment			x		
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)			x		
Environmental isotopes (incomplete)					
Monitoring borehole section					
Hydraulic effects (short circuiting)					

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KSH02 (to 1,001.11 m at an inclination of –85.67° to the horizontal) between 2003-03-03 to 2003-06-11, i.e. sample collected in 2003-03-12 and used here. Na-HCO_3 fresh groundwater with low chloride (6.3 mg/L) and low drilling water content (0.02%) with $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –78.8‰ VSMOW; tritium at 7.2 TU, ^{13}C at –17.45‰ PDB and ^{14}C at 55.73 pmC.

Charge Balance: Measured Sicada value at –0.80% (sample 5811 at –12.70% is omitted).

Time Series: Sampled on two occasions during the same day (2003-09-05) using the PLU hydraulic testing equipment; inadequate time series. Brackish groundwater with a stable salinity of 7,803–7,733 mg/L Cl; this stability is reflected by the other major ions. Drilling water is low and consistent at 1.48–1.53%. Major ions incomplete for the retained sample; no S^{2-}.

Trace elements: Reasonably good coverage.

Isotopes: Complete; no carbon isotopes (lack of HCO_3 ~ 5 mg/L). Tritium below detection (–0.8 TU) and $\delta^{18}O$ at –12.80‰ VSMOW suggesting a weak glacial component.

General: Na(Ca)-Cl(SO_4) brackish non-marine groundwater with a possible weak glacial component.

Comment: Despite the inadequate time series data, this groundwater is considered closely representative of the sampled depth level. Allocated Category 3.

D2.2.2 KSH02 (411.00–439.00 m; mid. vertical elevation: –418.66 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)			?		
Time series (adequate)					
Time series (inadequate)			x		
Time series absent					
Suitable section length					
Tube sampling					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)					
Environmental isotopes (incomplete)			x		
Monitoring borehole section			x		
Hydraulic effects (short circuiting)			x?		

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KSH02 (to 1,001.11 m at an inclination of –85.67° to the horizontal) between 2003-03-03 to 2003-06-11, i.e. sample collected in 2003-03-12 and used here. Na-HCO_3 fresh groundwater with low chloride (6.3 mg/L) and low drilling water content (0.02%) with $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –78.8‰ VSMOW; tritium at 7.2 TU, $\delta^{13}C$ at –17.45‰ PDB and ^{14}C at 55.73 pmC.

Charge Balance: Measured Sicada values at –3.69% to –0.42%.

Time Series: Sampled on three occasions (2005-11-18, 2006-06-27 and 2006-11-08) from a monitoring borehole; reasonable time series. Brackish groundwater showing instability (increase) in salinity (7,880–8,090 mg/L Cl) reflected by small increases in Ca and Mg and a decrease in SO_4. Drilling water is high at 16.20%, 17.50% to 10.80% with increasing time. Major ions incomplete for the selected second sampling occasion (no S^{2-}) and no Fe(tot), Fe^{2+}, S^{2-}, I and TOC/DOC for the other two sampling occasions.

Trace elements: Good coverage for the selected sample.

Isotopes: Incomplete; $\delta^{13}C$ at –21.38‰ PDB, no ^{14}C. Tritium below detection (–0.8 TU), and $\delta^{18}O$ at –12.80‰ VSMOW suggesting a weak glacial component.

General: Na(Ca)-Cl brackish non-marine groundwater with a possible weak glacial component.

Comment: Despite the inadequate time series data, this groundwater is considered closely representative of the sampled depth level, and corresponds to the previously described sample from approximately the same depth. Since there is a time lapse of over 2 years between these sampling periods, this further underlines the stability of the groundwater chemistry and supports the categories given. The high drilling water contents may have been influenced by hydraulic tracer tests using uranine carried out close to this present level (422.3–423.3 m) from 2004-09-02 to 2004-09-21, and therefore may have influenced all three sampling occasions. In addition, further tests were carried out at the 411.0–438.0 m level from 2005-11-23 to 2005-11-28 and may therefore have influenced the final two sampling occasions. Allocated Category 3.

D2.2.3 KSH02 (575.00–580.00 m; mid. vertical elevation: –570.90 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)			x		
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)			x		
Time series absent					
Suitable section length			x		
Tube sampling					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment			x		
Charge balance ±5% (±10% for <50 mg/L Cl)			x		
Major ions (complete)					
Major ions (incomplete)			x		
Environmental isotopes (complete)			x		
Environmental isotopes (incomplete)					
Monitoring borehole sections					
Hydraulic effects (short circuiting)					

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KSH02 (to 1,001.11 m at an inclination of –85.67° to the horizontal) between 2003-03-03 to 2003-06-11, i.e. sample collected in 2003-03-12 and used here. Na-HCO$_3$ fresh groundwater with low chloride (6.3 mg/L) and low drilling water content (0.02%) with δ^{18}O at –10.9‰ VSMOW and δ^{2}H at –78.8‰ VSMOW; tritium at 7.2 TU, ^{13}C at –17.45‰ PDB and ^{14}C at 55.73 pmC.

Charge Balance: Measured Sicada values at –4.31% to –1.06%.

Time Series: Sampled on two occasions during the same day (2003-09-15) using the PLU hydraulic testing equipment; inadequate time series. Brackish groundwater with a stable salinity of 8,245.5–8,262.3 mg/L Cl; this stability is reflected by the other major ions. Drilling water is low and consistent at 0.13%. Major ions incomplete for the retained second sample; no S^{2-}, although a value is recorded for the first sample that can be used.

Trace elements: Reasonably good coverage.

Isotopes: Complete; no carbon isotopes (lack of HCO$_3$ ~ 6 mg/L). Tritium below detection (–0.8 TU), and δ^{18}O at –12.99 to –12.90‰ VSMOW suggest s weak glacial component.

General: Na(Ca)-Cl(SO_4) brackish non-marine groundwater with a weak glacial component.

Comment: Despite the inadequate time series data, this groundwater is considered closely representative of the sampled depth level. Allocated Category 3.

D2.2.4 KSH02 (957.20–958.20 m; mid. vertical elevation: –950.41 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)				x	
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)				x	
Time series absent					
Suitable section length				x	
Tube sampling					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment				x	
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)				x	
Major ions (incomplete)					
Environmental isotopes (complete)				x	
Environmental isotopes (incomplete)					
Monitoring borehole sections					
Hydraulic effects (short circuiting)					

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KSH02 (to 1,001.11 m at an inclination of –85.67° to the horizontal) between 2003-03-03 to 2003-06-11, i.e. sample collected in 2003-03-12 and used here. Na-HCO_3 fresh groundwater with low chloride (6.3 mg/L) and low drilling water content (0.02%) with $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –78.8‰ VSMOW; tritium at 7.2 TU, $\delta^{13}C$ at –17.45‰ PDB and ^{14}C at 55.73 pmC.

Charge Balance: Measured Sicada value at –4.08% (second sampling no value recorded).

Time Series: Sampled on two occasions during the same day (2004-02-11) using the PLU hydraulic testing equipment; inadequate time series. Saline groundwater with a stable salinity of 16,800 mg/L Cl; this stability is reflected by the other major ions recorded. Drilling water is low and consistently < 1% (0.18–0.39%). Major ions complete for the retained first sample; second sample records only HCO_3, SO_4, Br, F, Fe(tot), Fe^{2+} and S^{2-}.

Trace elements: Good coverage for selected sample.

Isotopes: Complete; no carbon isotopes (lack of HCO_3 ~ 7 mg/L). Tritium below detection (–0.8 TU) and $\delta^{18}O$ at –11.00‰ VSMOW.

General: Ca(Na)-Cl(SO_4) saline non-marine groundwater.

Comment: Despite the lack of time series data, this groundwater is considered closely representative of the sampled depth level. Allocated Category 4.

D2.2.5 KSH02 (955.00–963.00 m; mid. vertical elevation: –951.71 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)	x				
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					
Drilling water (> 10%)					
Time series (adequate)	x				
Time series (inadequate)					
Time series absent					
Suitable section length	x				
Tube sampling					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					
Charge balance ±5% (±10% for <50 mg/L Cl)	x				
Major ions (complete)	x				
Major ions (incomplete)					
Environmental isotopes (complete)	x				
Environmental isotopes (incomplete)					
Monitoring borehole section	x				
Hydraulic effects (short circuiting)					

Drilling Water: HLX10 (3.00–85 m; mid. vertical elevation: –29.25 m). There is one documented drilling water sample in the Extended L.2.3 dataset from the time of drilling borehole KSH02 (to 1,001.11 m at an inclination of –85.67° to the horizontal) between 2003-03-03 to 2003-06-11, i.e. sample collected in 2003-03-12 and used here. Na-HCO_3 fresh groundwater with low chloride (6.3 mg/L) and low drilling water content (0.02%) with $\delta^{18}O$ at –10.9‰ VSMOW and $\delta^{2}H$ at –78.8‰ VSMOW; tritium at 7.2 TU, $\delta^{13}C$ at –17.45‰ PDB and ^{14}C at 55.73 pmC.

Charge Balance: Measured Sicada values at –0.18% to –0.66%.

Time Series: Sampled on three occasions (2005-11-18, 2006-06-27 and 2006-11-08) from a monitoring borehole; reasonable time series. Brackish groundwater showing instability (increase) in salinity (16,600–17,200 mg/L Cl) reflected by small increases in K and Ca and decreases in Na and SO_4. Drilling water is low and consistent (0.59–0.82%). Major ions complete for the selected second sampling occasion but Fe(tot), Fe^{2+}, S^{2-}, I and TOC/DOC are absent for the other two sampling occasions.

Trace elements: Good coverage for the selected sample.

Isotopes: Complete; no carbon isotopes (lack of $HCO_3 \sim 8$ mg/L). Tritium below detection (–0.8 TU) but at 0.84 TU for the selected sample, and $\delta^{18}O$ at –10.90‰ VSMOW.

General: Ca(Na)-Cl saline non-marine groundwater.

Comment: Despite the inadequate time series data and some evidence of instability, this groundwater is considered representative of the sampled depth level, and corresponds closely to the previously described sample from approximately the same depth. Since there is a time lapse of almost 2 years between these sampling periods, this further underlines the stability of the groundwater chemistry and supports the category given. Hydraulic tracer tests using uranine have been carried out in the same section from 2005-11-22 to 2005-11-28 and therefore may have influenced the second and third sampling occasions. However, the low drilling water content calculated would seem to argue against any major effect. Allocated Category 1.

KSH02: Tube samples sampled every 50 m from 00.00–941.00 m (2003-06-18) are considered unrepresentative and allocated Category 5.

D2.3 Description of Borehole KSH03A

Borehole KSH03A is 1,000.70 m long (vertical depth of 829.2 m), cased to 100.50 m, and inclined at –59.11° from the horizontal. The borehole was drilled from 2003-08-13 to 2003-11-07 and the main objectives were to gain geological information at depth of the eastern part of the Simpevarp peninsula and to facilitate further hydrogeological and hydrochemical investigations at this depth. Borehole KSH03A from about 100–180 m initially penetrates mostly fine-grained dioritoid and Ävrö granite containing some small pegmatite intercalations. From 200–280 m quartz monzodiorite dominates and, finally, homogeneous Ävrö granite dominates to the hole bottom containing only a few significant intercalations of fine-grained dioritoid, diorite gabbro and granite. From 100–180 m the rock is characterised by 3–5 open fractures/metre increasing markedly from 180–300 m where up to 20 open fractures/metre have been recorded accompanied by intense wall rock alteration/oxidation. From 300 m to the hole bottom the average open fracture frequency is 0–3 fracture/metre; exceptions include around the 860 m and 930–975 m levels where there is an increase to 5–10 open fractures/metre and only a slight alteration of the rock is observed.

References: SKB P-04-51, P-04-233, P-04-290, R-04-16, R-04-74. Discussion of the differential flow logging and hydrochemical logging data and their interpretation are presented in R-04-16 and R-04-74.

D2.3.1 KSH03A (00–40.00 m; mid. vertical elevation: –12.99 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)					
Drilling water (≤ 5%)					
Drilling water (≤ 10%)					x
Drilling water (> 10%)					
Time series (adequate)					
Time series (inadequate)					
Time series absent					x
Suitable section length					
Tube sampling					
Sampling during drilling					
Sampling using PLU hydraulic testing equipment					x
Charge balance ±5% (±10% for <50 mg/L Cl)					
Major ions (complete)					
Major ions (incomplete)					x
Environmental isotopes (complete)					
Environmental isotopes (incomplete)					x
Monitoring borehole sections					
Hydraulic effects (short circuiting)					x?

Drilling Water: HSH03 (0.00–103.00 m). There is one documented sample from the time of drilling borehole KSH03A to 1,000.70 m at an inclination of –59.09° to the horizontal from 2003-08-13 to 2003-11-07. In the Extended L.2.3 dataset the closest documented sample is from 2003-09-16 and used here. Na(Ca)-Cl(HCO_3) brackish meteoric groundwater with chloride at 462.9 mg/L. $\delta^{13}C$ at –17.80‰ PDB; ^{14}C at 61.00 pmC, tritium at 7.5 TU, $\delta^{18}O$ at –10.7‰ VSMOW and $\delta^{2}H$ at –76.1‰ VSMOW.

Charge Balance: Measured Sicada value unacceptable at –18.62% (sample 7086).

Time Series: Sampled on one occasion (2004-01-27); inadequate time series. Brackish groundwater with a salinity of 3,890 mg/L Cl; drilling water is high at 6.77%. Major ions incomplete; no Fe(tot), Fe^{2+}, S^{2-}, I and TOC/DOC.

Trace elements: Lack of data.

Isotopes: Incomplete; no carbon isotopes or tritium. $\delta^{18}O$ at –9.30‰ VSMOW.

General: Ca(Na)-Cl(SO_4) brackish groundwater mix.

Comment: Inadequate time series, unacceptable charge balance, incomplete major and isotope data and a long borehole section possibly facilitating mixing/short circuiting. This groundwater is not considered representative of the sampled depth level. Allocated Category 5.

D2.3.2 KSH03A (00–100.60 m; mid. vertical elevation: –38.73 m)

Cored Borehole Category	1	2	3	4	5
Drilling water (≤ 1%)				–	
Drilling water (≤ 5%)				–	
Drilling water (≤ 10%)				–	
Drilling water (> 10%)				–	
Time series (adequate)					
Time series (inadequate)				x	
Time series absent					
Suitable section length					
Tube sampling					
Sampling during drilling				x	
Sampling using PLU hydraulic testing equipment					
Charge balance ±5% (±10% for <50 mg/L Cl)				x	
Major ions (complete)					
Major ions (incomplete)				x	
Environmental isotopes (complete)					
Environmental isotopes (incomplete)				x	
Monitoring borehole sections					
Hydraulic effects (short circuiting)				x?	

Drilling Water: HSH03 (0.00–103.00 m). There is one documented sample from the time of drilling borehole KSH03A to 1,000.70 m at an inclination of –59.09° to the horizontal from 2003-08-13 to 2003-11-07. In the Extended L.2.3 dataset the closest documented sample is from 2003-09-16 and used here. Na(Ca)-Cl(HCO_3) brackish meteoric groundwater with chloride at 462.9 mg/L. $\delta^{13}C$ at –17.80‰ PDB; ^{14}C at 61.00 pmC, tritium at 7.5 TU, $\delta^{18}O$ at –10.7‰ VSMOW and $\delta^{2}H$ at –76.1‰ VSMOW.

Charge Balance: Measured Sicada values at –0.98% to +5.14%.

Time Series: Sampled on three occasions during the same day (2003-08-21) during the final stages of the percussion drilling; inadequate time series. Brackish groundwater showing unstable salinity during sampling from 644.4 to 329.3 to 510.0 mg/L Cl; instability is indicated by the other major ions. No drilling water recorded. Major ions incomplete; no Fe(tot), Fe^{2+}, S^{2-}, I and DOC.

Trace elements: Lack of data.

Isotopes: Incomplete; no carbon isotopes. Tritium at 8.8–9.9 TU and $\delta^{18}O$ at –10.0 to –9.8‰ VSMOW indicating a large modern recharge component.

General: Na(Ca)-Cl(HCO_3,SO_4) brackish groundwater mix.

Comment: Inadequate time series, uncertain drilling water content, incomplete major and isotope data, and a long borehole section possibly facilitating mixing/short circuiting. Despite these factors, this groundwater is considered to be reasonably representative of the sampled depth level. Allocated Category 4.

KSH03A: Tube samples sampled every 50 m from 90.00–940.00 m (2004-01-27) are considered unrepresentative and allocated Category 5.